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MINI-ASSESSMENT OF
ENVIRONMENTAL TRENDS AND PROBLEMS:
ALTERNATIVE FEEDSTOCKS

by

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16. ABSTRACT

This report discusses the potential for replacing oil and natural gas, the major organic chemical feedstocks, with alternative source materials and the consequent potential for environmental damage. Major emphasis is on five basic chemicals, and others are also considered in order to provide a more complete view of the chemical industry, particularly of those sectors where alternative feedstocks may have a significant impact. Using the Reference Materials System, current sources and uses of key chemicals are traced and a projection is made to the year 2000 under assumptions reflecting current market conditions. Three scenarios then define the upper limits for potential alternative feedstocks: (1) coal-based synthesis gas, (2) synfuel by-products, and (3) biomass. Residuals and socio-economic impacts are identified. Potential problems are ranked speculatively in terms of severity and then ranked in terms of likelihood. Several areas of further research are recommended. An extensive bibliography lists sources on the chemical industry and on fossil hydrocarbon and biomass derived feedstocks.

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FOREWORD

An effective environmental research and development program must be focused on the future as well as the present. The Office of Strategic Assessment and Special Studies has an ongoing responsibility to contribute to the effectiveness of EPA's research and development effort by assessing and expanding the state of knowledge in two basic areas:

- Information/data regarding future economic and technological trends; and
- Methodological development through which such trends are evaluated and meaningful projections made.

This report is a Mini-Assessment of the potential for future environmental disruption from the use of unconventional chemical feedstocks and of the consequent needs for future research. It summarizes the state of knowledge concerning the feedstock issue and defines it in terms of potential public health and environmental policy implications. Primary emphasis is placed on identifying gaps in the data, state of knowledge, and methodologies for assessing future trends and potential problems.

PREFACE

The methodological basis for this study derives from research performed by K.C. Hoffman and N. Bhagat at Brookhaven National Laboratory. This research aimed at deriving a network description of the flow of material resources from resource extraction through refinement, production and transportation processes to utilization, maintenance, and recycling operations. It was sponsored by the Committee on Renewable Resources for Industrial Materials (CORRIM) of the National Academy of Sciences and the principal research result is an analytical framework called the Reference Materials System (RMS).

The Brookhaven approach has been applied here in detail for the first time. The MATHTECH staff principally responsible for the results are Gordon M. Burck and Barrett J. Riordan, who worked under the tutelage of Kenneth C. Hoffman and were ably assisted by Richard W. Meehan II. MATHTECH wishes to acknowledge the contribution of three consultants who provided invaluable advice and criticism throughout the project. They are Paul N. Cheremisinoff, Associate Professor of Environmental Engineering at the New Jersey Institute of Technology; Ingemar Falkehag, Director of Renewing Systems, Inc.; and Irving S. Goldstein, Professor of Wood and Paper Science at North Carolina State University. The conclusions of this report, however, do not necessarily agree with those of these individuals and any errors or miscalculations are strictly the responsibility of MATHTECH, Inc.

In addition to the consultants, several EPA staff provided strong guidance to the study effort. Principal among EPA staff was Dr. David Bennett, the OSASS Project Officer, who devoted considerable time and thought to overseeing this project and contributed greatly to its success. Morris Levin, the OSASS Mini-Assessment Coordinator, was also most helpful. MATHTECH is also grateful to an additional number of EPA staff who commented upon progress reports and who carefully reviewed early drafts of the final report. Without their efforts the quality of this report would be much diminished.

ABSTRACT

The principal concern of this report is the potential for replacing oil and natural gas, the major organic chemical feedstocks, with alternative source materials and the consequent potential for environmental damage. The major emphasis is on five basic chemicals -- benzene, ethylene, cyclohexane, ethylbenzene and styrene -- selected as representative of all basic organics. Synthesis gas and other large volume basic chemicals, plus major derivatives, are also considered in order to provide a more complete view of the chemical industry, particularly of those sectors where alternative feedstocks may have a significant impact.

Using the Reference Materials System, current sources and uses of the key chemicals are traced and a projection is made to the year 2000 under assumptions reflecting current market conditions. Three scenarios are then defined describing the upper limits of potential alternative feedstock substitution for conventional oil and natural gas. The three substitutes chosen are (1) coal-based synthesis gas, (2) synfuel by-products, and (3) biomass.

Residuals from extraction and chemical processing and socio-economic impacts are quantified for each scenario. The potential problems are identified, ranked speculatively in terms of severity for specific EPA regions, and then ranked in terms of likelihood. Although the biomass scenario dominates the top of the severity list, when likelihood factors are also considered only nutrient and pesticide runoff retains its relative importance. Two other problems appear to be unambiguously more important: socio-economic impacts in the synfuel scenario (Region VIII) and total dissolved solids in the synthesis gas scenario (Region III).

Research is recommended on the locational determinants of the chemical industry; on means to monitor trace elements and toxic substances emitted by new chemical and energy plants; and on the environmental aspects of silviculture and lignin chemical processing.

This report is submitted in fulfillment of Contract No. 68-02-3639 by MATHTECH, Inc., under the sponsorship of the U.S. Environmental Protection Agency. This report covers the period October 10, 1980, to April 10, 1981, and work was completed as of April 10, 1981.

TABLE OF CONTENTS

Page

Forward.. iii
Preface.. iv
Abstract... v
List of Tables....................................... viii
List of Figures...................................... x
List of Abbreviations and Symbols.................... xi
SUMMARY.. xii

1. CHEMICAL FEEDSTOCKS AND ALTERNATIVE SOURCES: THE STATE OF KNOWLEDGE.............................. 1

  1.1. Introduction to the Chemical Industry.......... 1

  1.2. Major Basic Chemicals: Current Status.......... 7
    1.2.1. System R-1980.............................. 9
    1.2.2. Overview of Potential Feedstocks........... 10

  1.3. Alternative Future Scenarios................... 18
    1.3.1. Scenario Formulation....................... 18
    1.3.2. Scenario R-2000............................ 21
    1.3.3. Scenario A-1: Synthesis Gas From Coal.. 25
    1.3.4. Scenario A-2: Synfuel By-Products...... 28
    1.3.5. Scenario A-3: Biomass...................... 33
    1.3.6. Summary of Alternative Feedstock Futures............................... 38

2. ENVIRONMENTAL IMPACTS.............................. 50

  2.1. Introduction................................... 50

  2.2. Processing Phase............................... 53
    2.2.1. Aggregation of Residuals................... 53
    2.2.2. Regional Distribution...................... 63

  2.3. Resource Extraction Phase...................... 71
    2.3.1. Scenario A-1............................... 72
    2.3.2. Scenario A-3............................... 82

Page

3. CONCLUSIONS AND RECOMMENDATIONS.................... 93

3.1. Introduction.................................. 93
  3.1.1. Restatement of Objectives............... 93
  3.1.2. The Probability/Impact Interface........ 94

3.2. Overall Assessment of Environmental Impacts.... 95
  3.2.1. Key Environmental Issues................ 95
    (1) Severity Ranking.................... 96
    (2) Likelihood Ranking.................. 99
  3.2.2. Information Deficiencies................ 101

3.3. Initiating Events............................. 103
  3.3.1. The Futurescan Process.................. 103
  3.3.2. Events and Sequences.................... 105

3.4. Recommendations............................... 110
  3.4.1. Key Events.............................. 110
  3.4.2. Research Recommendations................ 111

APPENDICES

A. The Reference Materials System................ 114

B. Underlying Assumptions........................ 126
  B.1. Summary of Energy Scenario............... 126
  B.2. Federal Policy and Regulation............ 130

C. RMS Scenario Detail........................... 132
  C.1. System R-1980............................ 132
  C.2. Scenario R-2000.......................... 147
  C.3. Scenario A-1: Synthesis Gas.............. 156
  C.4. Scenario A-2: Synfuel By-Products........ 162
  C.5. Scenario A-3: Biomass.................... 169

D. Technologies for Alternative Futures.......... 179

E. Environmental Coefficients.................... 185
  E.1. R-1980................................... 185
  E.2. R-2000................................... 194
  E.3. A-1...................................... 197
  E.4. A-2...................................... 200
  E.5. A-3...................................... 200

F. Annotated Bibliography........................ 210

G. Conversion Factors............................ 234

LIST OF TABLES

Number		Page
S.1	Key Characteristics of Alternative Futures.......	xiv
S.2	Ten Prominent Environmental Concerns.............	xvii
S.3	Ten Important Areas of Information Deficiency....	xix
1	Importance of U.S. Chemical Feedstock Sources Relative to Total Energy Resource Consumption -- 1978..........................	4
2	Leading U.S. Organic Chemicals Production -- 1979	6
3	Synthetic Material Sectors......................	7
4	Five Basic Chemicals: Scenario R-1980 Summary..	11
5	Relative Availabilities of Feedstocks...........	17
6	Scenario R-2000 Summary......................	24
7	Scenario A-1: Synthesis Gas Summary.............	26
8	Scenario A-2: Synfuel By-Products Summary........	31
9	Scenario A-3: Biomass Summary...................	36
10	Summary of Entry Points into Chemical System.....	40
11	Key Characteristics of Alternative Futures.......	47
12	R-1980 Aggregated Residuals....................	54
13	R-2000 Aggregated Residuals....................	56
14	A-1 Aggregated Residuals....................	57
15	A-2 Aggregated Residuals....................	58
16	A-3 Aggregated Residuals....................	59
17	Summary of Residuals by Scenario................	60
18	Change from 1980 Baseline.......................	62

Page

19 Distribution of Basic Chemical Processing Capacity.................................. 64

20 Output of the Pulp and Paper Industry by EPA Region: 1975 and 2000...................... 69

21 Residuals from Underground Mining and Coal Cleaning................................... 75

22 Residuals from Western Surface Mining and Coal Preparation........................... 80

23 Comparative Fertilizer Inputs................. 87

24 Ten Prominent Environmental Concerns.......... 97

25 Ten Important Areas of Information Deficiency. 102

26 Eastern Coal (Regions III, IV and V) Scenario: A-1............................. 106

27 Western Coal (Regions VI & VIII) Scenario: A-1.................................... 107

28 Wood Products (Region IV) Scenario: A-3....... 108

B.1 U.S. Energy Consumption....................... 127

E.1 R-1980 Relevant Environmental Coefficients.... 193

E.2 R-2000 Relevant Environmental Coefficients.... 195

E.3 A-1 Relevant Environmental Coefficients.... 199

E.4 A-2 Relevant Environmental Coefficients.... 201

E.5 A-3 Relevant Environmental Coefficients.... 208

G.1 Conversion Factors........................... 234

LIST OF FIGURES

Number		Pages
1	Benzene Feedstocks Summary	41
2	Ethylene Feedstocks Summary	43
3	Chemical Industry Feedstock Source Summary	45
4	Severity/Likelihood Rank Order Matrix	100
A.1	Future Potential of Woodland, Agricultural, Municipal and Feedlot Residues for Chemical Use	120
A.2	U.S. Materials System, 1977	121
A.3	Reference Materials System	124
C.1	System R-1980	133,136-8,140-5
C.2	System R-2000	148-9,151-3,155
C.3	System A-1: Synthesis Gas	157-161
C.4	System A-2: Synfuel By-Products	163-8
C.5	System A-3: Biomass	171,173-7
E.1	Collected Benzene Trajectories	186
E.2	Collected Ethylene Trajectories	187
E.3	Cyclohexane, Ethylbenzene, Styrene Trajectories	188

LIST OF ABBREVIATIONS AND SYMBOLS

Abbreviations

BOD	biological oxygen demand
BTU	British thermal unit
BTX	benzene, toluene, and xylene
COD	chemical oxygen demand
CPI	chemical process industry
HC	hydrocarbons
kg	kilogram
kg mole	kilogram mole
MSW	municipal solid waste
Quad	quadrillion BTUs
RMS	Reference Materials System
SRC	solvent refined coal
TDS	total dissolved solids
TSS	total suspended solids

Symbols

C_1	one carbon hydrocarbon; methane
C_4	four carbon hydrocarbons
CO	carbon monoxide
H_2	hydrogen
NO_x	nitrogen oxides
P	probability
SO_2	sulfur dioxide

1. CHEMICAL FEEDSTOCKS AND ALTERNATIVE SOURCES: THE STATE OF KNOWLEDGE

This section attempts to set forth the current state of knowledge regarding potential commericial use of alternative feedstocks. It describes scenarios through which alternative feedstocks are developed, including their likelihood and magnitude. Principally, in conjunction with Appendices A through D, it sets forth an analytical framework useful for the examination of this question. Within this framework this section collects the important information existing in the technical literature.

1.1. Introduction to the Chemical Industry

Most chemical feedstocks are by-products of energy production and represent only three to four percent of total oil and natural gas consumed. The qualitative difference between the two industries is clear in the definition given in Kirk-Othmer:

> Petrochemical feedstocks are mainly hydrocarbons that are transferred from the energy sector to the chemical sector. ...they are transferred from operations commonly performed in preparation of usable energy to operations in which they are first used as raw materials in processes involving a chemical change or physical separation before eventual end use. (9)

The chemical industry has developed basically because of the strong incentives to use free or low cost energy by-products, and, with some exceptions, it remains in this subsidiary status. For example, ethylene, the leading organic chemical, became plentiful because ethane is produced as a by-product in fuel refineries. Whereas ethylene consumption (over 30 percent of basic petrochemicals) is about 13 billion kilograms per year, total gasoline use is about 300 billion kilograms per year. Similarly, natural gas liquids, the second largest feedstock source, were initially separated from gas to avoid pipeline condensation.

The products of the chemical industry are commonly referred to by the word "petrochemicals" which seems to imply "chemicals made from petroleum." In fact, crude oil supplies less than half of the feed material to the organic* chemical industry. Natural gas (methane) and natural gas liquids ("NGL"; mostly ethane, propane, and butane) supply 55 percent. While it is true that most natural gas is recovered along with crude oil from the same wells and is thus a coproduct of the oil industry, natural gas has been subject to different price regulations. It is also much less of a factor in international trade than is oil. Among U.S. energy sources, only natural gas liquids are committed as a chemical feedstock in excess of four percent of the total supply (see Table 1).

---

*While this report uses the terms "chemicals" and "chemical feedstocks" in reference to organic chemicals, it should be noted that organic (i.e., carbon-hydrogen bonded) chemicals are a small part of the total chemical industry. Among the largest volume chemicals in 1979, only ethylene makes the top ten, at number six, and propylene and benzene follow at 13 and 15. Ammonia (3), ammonium nitrate (12) and urea (14) appear in this report, but as products of synthesis gas from an organic source, not as organic chemicals themselves. Another energy sector qualification is that among the components of gasoline are tremendous quantities of propylene and benzene (about 9 and 90 billion kilograms per year), although in mixtures less pure than required for the chemical industry.

Not only is the relative contribution of oil versus gas subject to a variety of supply variables, but also the way in which a particular feedstock may contribute will change. In particular, there has been a steady change in the availability of various oil refinery streams for chemicals. Ethylene production in the United States has become increasingly based on heavier feeds such as naphtha, rather than the lighter ethane/propane feeds. (Naphtha has long been the standard feed material in Europe and Japan where less catalytic cracking of oil for gasoline is required and consequently less ethane is produced as a refinery by-product.) Whereas ethane-to-ethylene crackers produce a moderate number of by-products (e.g., acetylene, butadiene), naphtha crackers produce several times the weight of the principal product ethylene as by-products. This increases the challenge of marketing and makes production less flexible, but it also stimulates research to utilize newly abundant streams.

The source of chemical feedstocks, including coal and wood, relative to the energy industry is shown in Table 1. The table also shows the relative dependence of chemicals on each feed source. The future market share for each feedstock is the subject of this section. The contribution of each feedstock

Table 1. Importance of U.S. Chemical Feedstock Sources Relative to Total Energy Resource Consumption -- 1978

	Total U.S. Energy Resource Consumption			Sources of U.S. Chemical Feedstocks	
	Quads per year	Percent of total	Percent of Resource Consumed as Chemical Feedstocks	Quads per year	Percent of total
Coal	15	18.6	0.5	0.08	2.9
Natural Gas	20.4	25.3	3.4	0.70	26.1
Natural Gas Liquids	3.3	4.1	23.3	0.77	28.5
Oil	34.5	42.9	3.3	1.12	42.0
Other (including wood)	7.3	9.1	0.2	0.02	0.5
	80.5	100.0		2.7	100.0

"Quad" is shorthand for quadrillion (10^{15}) British Thermal Units equivalent to 1.055 x 10^{18} joules.

Sources: Appendix B.1; Reference 9

can be further divided. NGL is about one-half ethane and one-half propane/butane. Oil is about one-third aromatics (benzene, toluene and xylene, i.e., "BTX"), with the remainder olefins (e.g., ethylene, butadiene) and aliphatic species (e.g., paraffin). The feedstocks for 1978 total 2.7 Quads* or about 67 million metric-tons-crude-oil-equivalent (on an energy basis).

Table 2 shows the production of the leading organic chemicals for 1979 (average growth of 5.5 percent over 1978 production). This list totals about 70 million metric tons.** However, substantial amounts of some chemicals are, in turn, intermediates for other chemicals on the list - such as ethylene to ethylene dichloride to vinyl chloride, and benzene-plus-propylene to cumene to phenol-plus-acetone. There are also other smaller chemical products (e.g., cellulose from wood, naphthalene from coal tar) which are not derived from the primary chemicals on this list. The net production of the chemical industry is about 40 million metric tons. Major synthetic material divisions within that total are shown in Table 3. Other divisions include solvents, acids, agricultural chemicals, pharmaceuticals, and basic chemicals (e.g., benzene and toluene used in gasoline).

---

*A Quad is a quadrillion British Thermal Units, where a BTU equals 1,055 joules. Conversions to S.I. units are shown in Appendix G.

**A metric ton is 1000 kilograms.

Table 2. Leading U.S. Organic Chemicals Production -- 1979

Rank By Weight	Chemical	Production		Average Annual Change 1969-79
		10^6 kg	10^6 kg mole	
17	Acetic acid, synthetic	1,510	25	7%
19	Acetone	1,135	220	5
22	Acrylonitrile	916	17	6
32	Aniline	309	3.3	7
3	Benzene	5,755	74	4
37	Bisphenol A	261	1.1	12
16	1,3-Butadiene	1,611	30	1
30	n-Butanol	332	4.5	6
28	Caprolactam	429	3.8	na
15	Cumene	1,812	15	9
20	Cyclohexane	1,094	13	1
35	Dodecylbenzene	284	1.2	2
25	Ethanol, synthetic	593	13	-6
40	Ethanolamines	191	3.1	5
38	Ethyl chloride	259	4.0	-2
6	Ethylbenzene	3,869	36	6
1	Ethylene	13,239	472	6
5	Ethylene dichloride	5,362	54	7
12	Ethylene glycol	2,085	34	6
11	Ethylene oxide	2,394	54	4
42	2-Ethylhexanol	144	1.1	-2
10	Formaldehyde, 37%	2,924	97	4
24	Isopropyl alcohol	893	15	0
41	Maleic anhydride	161	1.6	6
9	Methanol, synthetic	3,362	105	6
39	Methyl chloride	204	4.0	1
33	Methyl ethyl ketone	294	4.1	3
31	Methyl chloroform	322	2.4	8
34	Methylene chloride	288	3.4	6
29	Perchloroethylene	349	2.1	2
18	Phenol, synthetic	1,336	14	6
27	Phthalic anhydride	471	3.2	3
2	Propylene	6,485	154	7
36	Propylene glycol	280	3.7	3
21	Propylene oxide	1,020	18	7
8	Styrene	3,395	33	5
13	Terephthalic acid, dimethyl ester	1,934	11	10
4	Toluene	5,370	58	8
23	Vinyl acetate	899	10	11
7	Vinyl chloride	3,422	55	7
26	o-Xylene	488	4.6	2
14	p-Xylene	1,894	18	10

Source: Chemical & Engineering News, 9 June 1980, p. 38.

Table 3. Synthetic Material Sectors

Group	Major Component Chemicals	Percent of Total Chemical Products
Thermoplastic Resins	polyethylene,-propylene,-styrene, -vinyl chloride,-amides	34
Thermosetting Resins	polyester, epoxy, urea, melamine, phenolics	6
Manmade Fibers	acetate, rayon, acrylic, nylon, olefins, polyester	12
Synthetic Rubber	acrylonitrile-butadiene-styrene, butyl, neoprene	3

Source: Chemical & Engineering News, 9 June 1980, p. 40.

Given the current situation, it is unlikely that alternative feedstock sources can be quickly substituted. They are subject to most of the same supply constraints as are petroleum and natural gas and will probably enter the economy much as these feedstocks did. Namely, the alternative hydrocarbons must first find a market as alternative fuels. Only then will intermediate (e.g., medium BTU gas in a high BTU plant) and by-product (e.g., lignin from trees-to-gasohol) materials be considered for their chemical potential.

1.2. Major Basic Chemicals: Current Status

Five principal organic chemicals were selected by EPA for detailed analysis. For each of these chemicals, a Reference Materials System (RMS) Chart displays that chemical's position in the current chemical industry (designated as

System R-1980) and additional RMS charts show the effects of four alternative feedstock futures. The organization, scope, and subsequent use of RMS charts are described in detail in Appendix A. The five principal chemicals and their associated chart numbers are:

Chart 1:	Benzene
Chart 2:	Ethylene
Chart 3:	Cyclohexane
Chart 4:	Ethylbenzene and Styrene

These chemicals were chosen to represent the vast array of basic organic chemicals. All are among the twenty largest volume organic chemicals (see Table 2). Ethylene and benzene are numbers one and three, while cyclohexane is number twenty. Ethylene and benzene are also primary chemicals - one chemical step removed from a feedstock. Ethylene is obtained by steam cracking of ethane or saturated hydrocarbon streams from refineries or from natural gas liquids. A substantial fraction of benzene is produced by dealkylating refinery toluene. Cyclohexane and ethylbenzene are secondary chemicals, i.e., one step removed from benzene. Styrene is a tertiary chemical obtained from ethylbenzene.

To present a more complete picture of the chemical industry and to include other chemicals that were judged to be important (in terms of changing feedstock patterns), additional RMS charts are included:

Chart 5:	Synthesis Gas (carbon monoxide and hydrogen), including methanol and (non-organic) ammonia; and

Chart 6: Other Basic Chemicals, including toluene, xylene, paraffins, naphthalene, acetylene, and propylene.

Complementing these six charts are four more that illustrate the chemical systems which might be built on the primary sources of alternative feedstocks, namely:

Chart 7: Coal and Peat;

Chart 8: Shale Oil, Tar Sands, and Heavy Oil;

Chart 9: Wood and Dry Biomass; and

Chart 10: Wet Biomass

The charts and a short narrative explanation are contained in Appendix C. The following sections highlight and summarize the chemical systems examined.

1.2.1. System R-1980

The set of charts for System R-1980 (see Appendix C.1) presents the average annual flows of the major organic chemicals during the years 1979 through 1981 and characterizes the chemicals in terms of current sources and markets. These data were primarily derived from published sources (13). In a few instances MATHTECH estimates are shown.

The flows are in millions of kilogram moles* and are intended to represent an internal balance rather than to match exactly any one year's production figures. Figures for an individual year can never be expected to balance, because:

---

*A kilogram mole (kg mole) is 1000 Avogadro Numbers (one Avogadro Number equals 6.025 x 10^{23}) of molecules, and it weighs in kilogram units the sum of the molecular weights of the component atoms. Kilogram moles, rather than weight units, are used on the charts to emphasize the distribution patterns. For instance, although over fifty percent more ethylene is used to make ethylene oxide than vinyl chloride, two chlorines weigh more than one oxygen and, on Table 2, vinyl chloride production is 1 2/3 times that of ethylene oxide. Feedstock sources which are not identifiable as specific chemicals will be quantified in terms of combustion energy (in BTUs or oil-equivalent).

- Chemicals may be stockpiled during market downturns, in anticipation of the planned shutdown of a plant for maintenance, or as insurance against an unplanned shutdown. Chemicals sold on long-term contracts must be delivered, even if they must be first purchased from a competitor;
- Chemicals which are not separated as salable products need not be reported to the Commerce Department. Thus, if several reaction steps take place in an integrated process, the volume of the intermediate can only be inferred. This is the case for ethylbenzene in benzene-to-styrene plants (Chart 4);
- Chemicals may go through a loop process, so recycle must be distinguished from net production. An example is acetic acid, which is converted to acetic anhydride. Acetic anhydride is in turn reacted with cellulose to form cellulose acetate, plus acetic acid which is recycled; and
- If only a few companies manufacture a chemical, they are not required to report their production in order to protect their competitive secrecy.

Table 4 summarizes the feedstock distribution for the selected chemicals in R-1980.

1.2.2. Overview of Potential Feedstocks

Among the potentially important feedstocks, some, such as some wood chemicals and coal chemicals, are well known. Many such sources were commercial prior to World War II and some remain so today. Other routes to petrochemical feedstocks are speculative at best, both in technological development and cost competitiveness.

Table 4. Five Basic Chemicals: Scenario R-1980 Summary

Feedstock	Total Source Consumption	Distribution of Key Chemicals by Feedstock				
	10^{12} BTU/yr	10^6 kg mole				
		Benzene/ Total BTX*	Ethylene	Cyclohexane	Ethyl- benzene	Styrene
Refinery Products	1240	67/127	180	-	3	small
Natural Gas						
Methane	770	-	-	-	-	-
Liquids	840	-	280	-	-	-
Coal Products						
From Coking	85	5/6	-	-	-	-
Synthesis Gas	-	-	-	-	-	-
Wood Pulp By-Products	15	-	-	-	-	-
Derivatives	-	0/3	-	13(benzene)	34	34
	2950	72/136	460	13	37	34

*BTX is benzene, toluene and xylene

Alternative feedstocks may impact the basic chemical system at a myriad of points. In particular, ethylene and benzene are major derivatives of several alternative feedstocks. Hence, if styrene endures, it could be entirely based on wood (an ironic turn of events for the displacer of paper cups). On the other hand, if that new dependence causes styrene to be relatively more expensive than other chemicals with similar properties, styrene production could decline sharply. Other chemicals may displace current intermediates, such as furfural (from xylose, Chart 9) for butadiene.

An important set of "coproducts" which could be particularly important contains phenol and acetone, minor by-products from shale oil processing but potentially major derivatives of wood processing. An alternative route to only one of them must cope with the market for the other.

Another point to note is that the alternative chemical sources will not necessarily cooperate in producing the starting materials to which the chemical processing industry is accustomed. For instance, synthesis gas may in the future supply the short chain hydrocarbons (via, e.g., the Mobil process) which now come from natural gas liquids and refinery by-products. More disconcerting for formal chemical use trees, some of the directions may be reversed. Two major examples will illustrate. At present, benzene is produced directly in the refining of crude oil or coal tar, or by the dealkylation of toluene which comes from the same sources. Its second largest use is to make phenol and acetone. In the future, phenol may be widely available from alternative sources (c.f., Chart 9) and could easily be reduced to benzene, which could then be alkylated to toluene, an original source, and xylene. Furthermore, phenol could be used to make aniline and nylons, current benzene derivatives (Charts 1 and 3). Thus, phenol could displace a significant amount of the demand for benzene as well as offer a new supply.

As a second example, ethanol is predominantly made by the hydration of ethylene. Although beverage liquors are still made by fermentation, synthetic alcohol is used in many food products such as vinegar, mustard and pickles, as well as for petrochemicals. However, in the future, ethanol derived by fermentation could supply the ester and ether reactions (Chart 2), regain its former uses such as acetaldehyde and butadiene, and even be dehydrogenated to ethylene, the prior source.

Every industry forecast of the feedstock future lays great emphasis on chemicals as being dependent on, or the "tail end"(3) of, the fuel industry. The consensus seems to be that competition will become more intense but that sufficient feedstocks from oil and natural gas will be available (4,16). The progressive shift to oil-based olefins (i.e., ethylene) plants puts olefin feedstocks in more direct competition with gasoline (20), while aromatics are competing with the need for octane boosters (1).

Synthesis gas generally appears attractive for some applications, particularly for oxygenated compounds. Synthesis gas will have greater potential as more single-product processes are developed. Just as the cracking of naphtha to ethylene produces many side products, Fischer-Tropsch hydrogenation of carbon monoxide produces a variety of hydrocarbons and alcohols or acids. The subsequent separations require both capital and energy, and suitable markets for all of the products. Economic uses for the large carbon dioxide by-product (25 percent or more of the carbon) from synthesis gas plants would also give a boost to this route (3), but the timing for a major synthesis gas industry remains in the late 1980s (4,23). One industry spokesman has predicted that as much as fifteen to thirty percent of all ethylene or its derivatives could be derived from coal-derived synthesis gas by 2000 (5). Another source predicts that all ethylene and propylene based chemicals could be produced from coal by 2000 (2).

Synfuels by-products will not begin to be available for many years nor to be significant until the end of the century. The immense investment and the sheer number of years necessary to carry out such an effort are impediments (11). The Energy Information Administration considers the oil shale program more likely to be successful than coal liquefaction (see Appendix B.1), whereas others dismiss oil shale outright as uneconomic. Industry opinions vary from "the high quality of shale oil could retard development of processes from synthesis gas because of superior economics with shale oil (3)" to "there is no special merit in shale oil as a chemical feedstock" and "synthetic crude oil from coal, however, is a better posibility (23)."

Biomass is primarily seen as a long term prospect. However, the increased interest in using C_4 compounds in place of benzene and other aromatics (4) may prepare the way for the large amounts of furfural that may become available from biomass.

The chemical industry is currently attempting to reduce total fossil energy consumption and move from heavy dependence on natural gas and fuel oil for energy to coal boilers equipped for co-generating electricity (11). As this and other demands for heavy fuel oil are reduced, refineries will have an incentive to crack or pyrolyze residual oil for ethylene and other chemicals. Further, due to other demands and constraints, refinery capacity and naphtha/gas oil production will not increase sufficiently to match ethylene demands on the currently common feedstocks. At the same time, available crude oil will continue to grow heavier in gravity, yielding a larger percentage of residual oil from each barrel. The technology is well developed and several companies have begun to crack whole crude oil directly to olefins (10,20). This latter trend will decrease the close competition with gasoline for refinery products.

In summary,

> Petroleum will continue to be the best source of olefin feedstock through the rest of this century, but it must always be kept in mind that it is a limited resource that must be conserved and will eventually run out. Industry must look forward to the use of coal, tar sands and biomass for its longer range needs. (20)

The first industry priority will be to use existing sources more creatively and efficiently, with even more recycling of chemical products such as contaminated solvents. But as supplies dwindle and energy explorations yield new potential feedstocks, transitions are likely to take place in an orderly evolution, rather than in a sudden revolution.

It is our judgment that a twenty year time scale is reasonable for comparing alternative feedstock sources. The scenarios below correspond to each phase -- oil-as-usual, synthesis gas, synthetics, biomass. They are all given for the year 2000, but the actual year when each might achieve its technical potential will vary according to the many factors discussed elsewhere in this report (see Appendix B.2). Thus the scenarios are not forecasts for 2000 or any other year, but they are compared against the demand for chemicals that may reasonably exist then.

None of the current feedstocks to the chemical industry will vanish by 2000 -- oil and gas availability is expected to decline only fifteen to twenty percent; although nations with lower production costs may attract new chemical production capacity. Nor will chemical feedstock demand begin to saturate the market for any available source -- only natural gas liquids will be used over the fifty percent level for chemical feedstocks, while oil and gas might contribute ten percent of their total production to chemicals.

On the other hand, were circumstances to change greatly, any of several alternative sources could conceivably supply the entire demand for chemicals. Table 5 shows that two to six times the chemical demand could be achieved from the various alternative sources with major effort.

Table 5. Relative Availabilities of Feedstocks

(10^{15} BTU)

	1980	2000 (est.)
Chemical Feedstock Demand	2.7	6.4
Alternative Feedstock Sources		
Coal, total	20	38*
Shale & Coal based synthetics	0	12*
Wood & Biomass	4	25*

*Forecasts of the upper limits of availability.

The major questions concern the interrelated issues of extracted material price, the cost and availability of transformation technology, the environmental impacts of transformation, and, in addition, the politics of competing demands. The ultimate outcome may be that synfuels, biomass, garbage, peat and other sources will indeed be used as fuel, as current research indicates, leaving the chemical industry a greater portion of the oil and gas it is accustomed to processing.

1.3. Alternative Future Scenarios

1.3.1. Scenario Formulation

A major component of this Mini-Assessment is the analysis of future trends in the use of alternative feedstocks for chemicals. These are presented in the form of scenarios covering the 1980 to 2000 period with the growth of markets and substitution trends between competing feedstocks represented in the format of the Reference Materials Systems.

In developing these scenarios, two options were considered:

- The development of an integrated and internally consistent chemical market and feedstock forecast consistent with overall economic growth: a demand oriented scenario; and
- The definition of potential roles and availability of alternative feedstocks and of potential markets that they might capture: a supply oriented scenario.

Early investigation indicated that reliable forecasts of chemical markets were not available for the year 2000 time frame, and that, in addition, the chemicals industry and the routes from feedstock to final products are so interconnected that a significant differential demand at the feedstock level would be difficult to conceive, much less achieve. Even booms for certain final products hardly affect the overall chemical markets. For instance, ten million electronic games each containing two pounds of polystyrene would add only 0.1 to the chart flows in millions of kg moles. The Federal ethanol program might in 1990 consume the equivalent of half of current chemical feedstocks, but it will be supplied directly from an alternative feedstock and thus not affect the demand for current chemical feedstocks (see Scenario A-3). A movement by the end of the century to automobiles made fifty percent of plastic would add perhaps five percent to year 2000 chemical products demand. But this demand would be spread over a diverse and interchangeable array of intermediates and would little affect the pattern of feedstock growth. Thus, demand oriented scenarios are both difficult to define and not enlightening at the level of basic chemicals.

The alternative of defining a supply-oriented scenario in terms of reasonable limits to the market penetration of new feedstocks and associated processes appears better suited to the needs of the Mini-Assessment. A supply-driven scenario assumes that a major alternative feedstock source becomes available and is fully used in the assumed quantity. In several cases, particularly in discussing synthesis gas (Scenario A-1), certain market penetration levels are assumed based on new process technology. But changes in final uses have not been considered as the key for entry for one or another alternative feedstock.

Another aspect of scenarios focusing on "feedstocks for basic chemicals" is that new hydrocarbon sources and primary products must "plug-in" to the existing system, producing the basic building block chemicals. This leads to study of the environmental impacts associated with the necessary conversions. It is more difficult to map the changes if several of the primary products, (e.g., ethanol and phenol from wood) take over as the basic building blocks, with the previous building blocks becoming smaller volume derivatives (see Section 1.3.5).

Alternatives which would replace the existing chemical industry with wholly new chemistry and products (e.g., sugar polymers) cannot be addressed because the basic chemicals would not be involved. The Reference Materials System is capable of handling such "structural change" scenarios, but such an effort is beyond the scope of a Mini-Assessment.

The scenarios presented here represent what are believed to be reasonable upper limits on the level of market penetration of those alternative feedstocks which may be anticipated. Exploring the upper limits most effectively points up major environmental concerns. The scenarios also imply the continued vitality and evolution of the U.S. chemicals industry, although at lower growth rates than historical levels. Determining which source will supply a given feedstock at a given future time is more difficult than investigating the effects whenever the change takes place. Further, many of the new processes identified are in an early development stage and cannot be completely characterized at this time.

Other uncertainties deal with the geographical location and extent of impacts and a range of technical and economic factors (see Appendix B.2). Political decisions, both domestic and foreign, taxes and subsidies, environmental and price regulations, and changes in the overwhelmingly larger fuel industry (which also depends on the above factors) all will affect feedstock availability and choice. To the extent possible, the scenarios that follow incorporate these uncertainties explicitly.

1.3.2. Scenario R-2000

Scenario R-2000 is one alternative future for the chemical industry, representing business-as-usual. As such, it is the most likely of the scenarios presented here. But even so it is highly speculative, quantitatively. That is, the numbers shown on the charts, representing demand for the basic chemicals in the year 2000, could vary by tens of percent in either direction. Nevertheless, the scenario as presented in the System R-2000 charts (Appendix C.2) is internally consistent and serves as a base for tracing and comparing the effects of alternative feedstocks. It provides both sufficient time for alternative feedstocks to make a significant contribution and sufficient scale to allow the identification of significant environmental impacts.

R-2000 is based on the following major assumptions:

1. Refined oil products will be available to the Chemical Process Industry (CPI), as necessary, through the end of the century; that is, the CPI will be able to outbid fuel users for its essential feedstocks. Since the value of a barrel of oil is increased several times on conversion to high volume plastic polymers, ten times when made into fibers,

and even one hundred times if converted to specialty chemicals (16), the use of oil for chemicals will remain attractive. Other factors, though not essential to R-2000, would mitigate a supply conflict. First of all, the Federal synthetic fuel program is assumed to be successful. Liquid fuels and therefore possible refinery feedstocks will be supplied up to one-third (six million barrels/day) by coal liquefaction and shale oil recovery. Secondly, refinery gasoline demand will decline ten percent, supplemented by ethanol production of 11-12 billion gallons per year.

2. Natural gas (methane) and natural gas liquids (NGL: ethane, propane, butane) will be available to the CPI at the present supply rate through the end of the century.

3. The refining industry will continue to cope successfully with the progression from NGL to increasingly heavy oil feedstocks in meeting the respective chemical demands.

4. Coal coking by-products will rise at the rate of GNP growth, two to three percent per year.

5. All new synthesis gas demand will be supplied by coal, primarily taking over non-ammonia production. Users requiring hydrogen rich gas will stay with methane. Coal-based synthesis gas will have by-products of ethylene and benzene.

6. There will be no important net import or export of chemical feedstocks or basic chemicals. In other words, this scenario is isolated from foreign competition and markets.

7. Chemical product demand to the end of the century will follow roughly the growth rates for the next five years, as

projected by several marketing services (13). Overall, the CPI grew at double digit rates in the 1950s and 1960s and at six percent in the 1970s. Chemical growth is projected to continue at about 3.5 percent until 2000. A variety of projections have recently appeared in trade literature: four percent growth in the 1980s (21), aromatics growth of one percent above GNP or three to four percent growth in the 1980s (1), ethylene growth of four to five percent to 2000 (20), or total growth of one and a half times that of the GNP.

Thus chemicals will still grow ahead of GNP, but now as commodities rather than as new materials, which previously displaced metals and wood in many functions and created novel products based on their own properties. At 3.5 percent growth the demand for basic chemicals will about double by 2000.

A few "high flyers" remain with near-term growth rates of ten percent (e.g., bisphenol-A on Chart 1, 1,4-butanediol on Chart 6, and vinyl acetate on Chart 2). But even these products will mature and their total weight production in 2000 may be only one-fifth of the growth in ethylene from 1980 to 2000.

As summarized in Table 6, the total feedstock demand in Scenario R-2000 will grow from 3.0 Quads in 1980 (Table 4) to about 6.4 Quads, or a growth of 3.8 percent per year. Synthesis gas from coal will grow to a 15 percent share from a base of zero. But the largest absolute growth will be the

Table 6. Scenario R-2000 Summary

Feedstock	Total Source Consumption 10^{12} BTU/yr	Distribution of Key Chemicals by Feedstock 10^6 kg mole				
		Benzene/ Total BTX	Ethylene	Cyclohexane	Ethyl- benzene	Styrene
Refinery Products	3680	111/230	775	-	8	small
Natural Gas						
Methane	770	-	-	-	-	-
Liquids	840	-	215	-	-	-
Coal Products						
From Coking	120	9/10	-	-	-	-
Synthesis Gas	930	25/27	85	-	-	-
Wood Pulp By-Products	20	-	-	-	-	-
Derivatives	-	0/3	-	18	85	90
	6360	145/270	1075	18	93	90

tripling of crude oil derived chemical feedstocks, a growth rate of 5.6 percent per year, to a 58 percent share.

1.3.3. Scenario A-1: Synthesis Gas From Coal

The R-2000 charts showed a rapid growth of synthesis gas (CO and/or H_2) in a portion of the ethylene derivative domain, with the growth supplied by coal. In this alternative future, coal captures from methane the total synthesis gas supply. Synthesis gas technology captures three ethylene derivatives: ethylene glycol, ethanol, and part of styrene. For styrene, half of the toluene that was dealkylated to benzene under R-2000 is transformed into styrene by a different route featuring carbonylation. Synthesis gas is also the basis for the assumed growth of methanol to five percent (by energy content) of the gasoline market either directly (ten percent by volume or 8.4 billion gallons per year) or as gasoline from the Mobil process. Besides its new uses, synthesis gas from coal also generates major byproduct flows of ethylene and aromatics (here assumed as an additional ten percent of the synthesis gas carbon into each by-product).

These changes in the basic chemical system are shown in larger type in the Reference Materials System A-1 Charts 1, 2, 4, 5 and 6, contained in Appendix C.3. The contributions of synthesis gas to total feedstocks and to the key chemicals are summarized in Table 7. There is also the potential for producing longer chain olefins, via the OXO, Mobil or Fischer-Tropsch processes (17), but such production would not directly

Table 7. Scenario A-1: Synthesis Gas Summary

Feedstock	Total Source Consumption 10^{12} BTU/yr	Distribution of Key Chemicals by Feedstock 10^6 kg mole				
		Benzene/ Total BTX	Ethylene	Cyclohexane	Ethyl-benzene	Styrene
Refinery Products	3290	53/196	400	-	8	small
Natural Gas						
Methane	380	-	-	-	-	-
Liquids	840	-	280	-	-	-
Coal Products						
From Coking	120	9/10	-	-	-	-
Synthesis Gas	1650	-	-	-	-	-
Methanol Fuel	960	-	-	-	-	-
By-Products	420	55/61	185	-	-	-
Wood Pulp By-Products	20	-	-	-	-	-
Derivatives	-	0/3	-	18	85	90
	7680	117/270	865	18	93	90

affect the basic chemicals.

As the role of synthesis gas expands, there may be contributions from the in-situ gasification of shale oil, wood or peat pyrolysis, or wood or municipal solid waste (MSW) partial oxidation. But the major near-term use in the CPI is more likely to be as a fuel in combined-cycle power plants, providing both electricity and steam to the chemical plant (11). The chemical industry uses more fuel than it does feedstocks, although conservation efforts have decreased fuel use dramatically in recent years, and improved catalytic processes should continue to be more efficient in their energy, as well as feedstock, requirements. Nevertheless, additional price incentive and technological opportunity for change of source remain.

The advent of a major high-BTU coal gasification industry would give a major impetus to synthesis gas from coal. A high-BTU plant is essentially only a methanation reactor attached to a medium-BTU synthesis gas plant. Consequently, chemical uses for syngas would share economies of scale in developing, design and manufacture of solids handling, pressurized feeding, and gas cleaning systems. Further, the availability of huge synthesis gas streams would encourage establishment of small adjacent chemical users and provide economies of scale on operating costs. For instance, the proposed Great Plains gasification complex will make its own methanol on site.

A restraining force on coal-based gas will be the shift of natural gas away from electricity generation and toward cleaner uses such as chemicals. Further, clean-burning gas should be replaced by coal in cement kilns and copper smelters (where sulfur is added to the combustion products as a smelting aid).

1.3.4. Scenario A-2: Synfuel By-Products

This scenario is totally dependent on Federal alternative energy programs and their potential by-products. A major premise of this study is that since mining, resource transportation and energy plant processing will be carried out solely to meet energy demands, environmental consequences of those activities must be faced and solved by the energy industry. The chemical industry should only be responsible (in analytical terms) for what it does after accepting a by-product stream.

For the most part, the development of a chemicals industry due to synfuels has been ignored. A 1975 study for the National Science Foundation, however, showed that BTX and naphthalene could be recovered economically from syncrude compared to twelve dollars per barrel* oil (17). Despite major oil price increases, however, industry is unlikely to pursue such technology until the syncrudes are flowing.

The Federal Synthetic Fuels Program calls for coal liquefaction output of 0.5 million barrels per day by 1987 and two million by 1992 (6). Shale oil is expected to provide 0.4 million barrels per day by 1990. The synthetic crude oil from these processes (plus solid boiler fuel from some) is the primary factor in energy studies. Economic analyses do consider by-products, such as ammonia, sulfur, and light hydrocarbons, but the implicit assumption is that they will be readily absorbed by the market with no volume or location impact. The major EPA study "Energy From the West" (22) shows huge liquefaction facilities connected to the outside world only by water and coal deliveries and a product oil pipeline.

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*A barrel is equivalent to 0.1590 cubic meters.

This scenario is a crude projection of by-products from the Federal program, but the scale of the result indicates what industrial impact might be expected. Assume that the Federal program meets its schedule and that its success will lead to further growth through the 1990s. In 2000, the United States could be producing one million barrels per day of shale oil and five million barrels per day of coal-derived fuels. When added to the ethanol program (0.7 million barrels by 1990), this would approximately replace present oil imports. Coal gasification to substitute for natural gas is not considered here. However, by-products as in scenario A-1, or even the entire scenario, could be added.

There are many coal conversion projects being developed and many reports on each. For this scenario, we have assigned half of the planned coal derived fuel each to Coal Oil from

Occidental's Catalytic Hydrocracking (15) and to the combined Light Refinery Liquids and Solvent Refined Coal from Gulf's SRC-II process (7). The cited references also give preliminary by-product expectations. Shale oil products are based on a widely cited conceptual shale oil refinery (8). The locally available by-products will depend on whether raw or partly refined shale oil is pipelined to a refinery (17). Detailed results would vary if other processes had been chosen, after an extensive investigation of technical and economic feasibility, but the scale of the result would be similar. And it is the scale which is the most striking and heretofore unrecognized finding of this scenario.

The outcome is summarized on Table 8 and shown on the Reference Material System Charts in Appendix C.4. The new coal-based synthesis gas uses assumed in Scenarios R-2000 and A-1 could be eroded in A-2 beyond the by-product ammonia displacement shown. Synfuel by-product methane might be made into synthesis gas considerably more cheaply than grass-roots gasified coal. However, the control of the synfuel by-product flow will no longer be in the chemical plant's hands; the plants will not be as predictable or flexible as refineries. Changes in coal feed and, hence, product distribution may not be communicated, the much larger and more complex synfuel plant will be more prone to upset, and overall the total synfuel plant production will respond to different market forces than the chemical plant does. These factors will inhibit new users of LPG and of the other by-product

Table 8. Scenario A-2 Synfuel By-Products Summary

Feedstock	Total Source Consumption 10^{12} BTU/yr	Distribution of Key Chemicals by Feedstock 10^6 kg mole				
		Benzene/ Total BTX	Ethylene	Cyclohexane	Ethyl-benzene	Styrene
Refinery Products						
Crude Oil	1260-1800	93/207	250	-	8	small
Synthetic Oil	540- 0					
Synfuel By-Products						
Liquid	2720	13/15	750	-	-	-
Methane	770(+excess)	-	-	-	-	-
Ammonia	100	-	-	-	-	-
Natural Gas	-	-	-	-	-	-
Coal Products						
From Coking	120	9/10	-	-	-	-
Synthesis Gas	830	22/24	75	-	-	-
Wood Pulp By-Products	20	-	-	-	-	-
Derivatives	-	0/3	-	18	85	90
	6360	137/259	1075	18	93	90

organics (fifty trillion BTUs) from committing themselves.

There are a multitude of restraints on synfuels development for energy purposes, the most discussed being the huge capital investment and the environmental impacts of mining and water use in the West. If the products are actually intended to contribute to the gasoline supply, rather than only to fuel oil and utility boiler fuels, then their behavior in an oil refinery must also be considered. None of the alternative or synthetic oils have any special merit as a refinery feed. In general, they (especially liquefied coal) have a lower-than-oil hydrogen content and consequently a lower potential for aliphatic products (ideally, octane). On the other hand, the potential for aromatics would be better, partially balancing the preponderance of short chain hydrocarbons in the synfuel by-products (17).

The choice of refining at the plant site or of transporting the synthetic oils to existing refineries, along with the subsequent use of the by-products in chemical operations, must also be faced. Since these are increasingly heavier oils, the variety and quantity of refinery by-products will increase as well. They will favor transport of the oil to existing integrated chemical complexes (primarily Gulf Coast) rather than construction of new refineries at the shale retort or coal liquefaction site (18).

If the chemical plants are built at the synfuel site, the environmental impacts would primarily be increased population and land and water useage. A chemical plant itself in, say, Wyoming would be essentially the same as on the Gulf Coast, but a few engineering changes such as the type of cooling (14) and amount of storage needed could make a difference environmentally. And, while any chemicals released would themselves be the same, the ambient conditions might be affected differently.

In summary, rigorous use of synfuel by-products could restrict oil refining to chemicals severely, impede the growth of coal based synthesis gas plants, and displace all natural gas based methane and liquids. Alternatively, the organic by-products could be used totally for plant and external fuel purposes.

1.3.5. Scenario A-3: Biomass

The final scenario involves a major transformation of feedstock acquisition to renewable sources. This alternative future is based on the total refining of trees to chemical components, using separation, hydrolysis, fermentation, standard refinery molecular processes, and pyrolysis gasification. Some pyrolysis of municipal solid waste (MSW) is included both as a supplemental source and as a comparison. Ethanol from corn is not discussed. That production is dominated by fuel demand and, further, it presents a food versus fuel question that cannot be adequately discussed here. (USDOE and USDA publications are listed in the Bibliography, Appendix F.)

The parts of wood which are subject to chemically distinct processing are cellulose (50 percent), hemicellulose (25 percent) and lignin (25 percent). In a prehydrolysis step, much of the hemicellulose is dissolved out of the wood. Then, in a second hydrolysis step, cellulose is converted to glucose, leaving a lignin residue along with the remaining hemicellulose. The hemicellulose is divided into six-carbon mannose (predominantly from hardwoods) which is combined with glucose from cellulose for further processing and into five-carbon xylose (predominantly from softwoods). Xylose and lignin are processed separately. Details are given in Appendix C.5. Development of the chemistry used to fragment and convert lignin is much less advanced than for cellulose chemistry, and thus the products and their quantities are more speculative. However, the lignin chemistry is the major key to making this scenario economically viable.

The Reference Materials System A-3 charts (see Appendix C.5) represent the use of 230 billion kg per year of dry wood, equivalent to the present consumption in the forest products industry. The total annual unused increment of forest biomass (the growth of forest plants which are never harvested but make the full cycle from seedlings to decayed matter) is about 700 billion kg per year (19). This quantity of wood may be supplied, along with expected growth in the existing forest products industry, by more complete harvesting in logging operations, more intensive management of natural forests, and efficient use of mill wastes. Or silviculture tree farming may eventually be used to ensure large and stable supplies.

There will also be a synthesis gas contribution from municipal solid wastes. The report assumes a total of 10,000 tons* per day of MSW (25 percent moisture; 24 percent metal, glass and other non-combustibles), pyrolyzed at one plant in each of four large metropolitan areas. At 8.4 kg mole of synthesis gas per ton of MSW, these plants would produce 54 million kg moles per year, probably converted to methanol in an integrated facility (12).

These flows are summarized in Table 9 and the System A-3 Charts in Appendix C.5.

The U.S. ethanol program will require four billion gallons per year of ethanol from cellulose, or approximately 260 million kg moles, which is about one-third of the wood-based potential in this alternative. While wood can saturate the chemical market for aromatics, the two-thirds of the ethanol available for chemicals can provide less than half of the ethylene (at the very conservative fermentation yields assumed). On the other hand, the synfuel by-products are BTX lean, so there is some natural complementarity of Alternatives 2 and 3.

In contrast, there is little complementarity with coal syngas scenarios. The wood-derived synthesis gas, plus the by-products methanol and light hydrocarbons, totally displace the coal-derived syngas used in R-2000.

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*A ton is equivalent to 907.2 kilograms.

Table 9. Scenario A-3: Biomass Summary

Feedstock	Total Source Consumption 10^{12} BTU/yr	Distribution of Key Chemicals by Feedstock 10^6 kg mole				
		Benzene/ Total BTX	Ethylene	Cyclohexane	Ethyl-benzene	Styrene
Refinery Products	1400	-	137	-	-	-
Natural Gas						
Methane	770	-	-	-	-	-
Liquids	840	-	280	-	-	-
Coal Coking	120	9/10	-	-	-	-
Wood						
Cellulose						
Chemicals	2260	-	450	-	-	-
Ethanol Fuel	830	-	-	-	-	-
Lignin						
BTX & Derivatives	830	86/204	-	18	8	-
Other Chemicals	520	-	137	-	-	-
Synthesis Gas	400	-	-	-	-	-
By-Products	60	-	44	-	-	-
MSW Synthesis Gas	10	-	-	-	-	-
Derivatives	-	0/3	-	-	85	90
	8040	95/217	1048	18	93	90

MSW-based synthesis gas plants would further displace coal. However, such plants will operate at a competitive processing disadvantage to wood-based plants in that they must deal with multiple impurities, in particular chlorine from PVC, which will pollute the product gas and interfere with the shift reaction catalyst. On the other hand, garbage may be an even cheaper feedstock than excess lignin, at least in the long run. In the shorter term the ethanol fuel program will be generating 18.5 million tons of lignin per year (nearly equal to the 20 million tons now burned in pulp and paper processing) plus bark and other wastes. If ethanol receives a large subsidy, this material could be essentially free for the hauling, as is garbage, and easier and cleaner to burn.

A major consequence of a large scale return to biomass could be a change in what is a "basic" chemical. At present, benzene and ethylene are the basic building blocks of the chemical industry. The mass of just these two chemicals is nearly fifty percent of the mass of all finished chemical products, and the charts have shown their complex connections in the chemical system.

However in Scenario A-3 phenol and ethanol, which are now derived from benzene and ethylene and hence oil and gas, could become primary products of wood processing and replace benzene and ethylene to become the building blocks of the future chemical industry. Thus the future focus of work on "alternative feedstocks for basic chemicals" might better be placed on the "feedstocks" or even "sources" than on the present-day "basic" chemicals, allowing "structural change" rather than "plug-in" scenarios and projections.

This scenario is at least twenty years into the future, farther than Scenarios A-1 and A-2. However, near-term attention should still be paid for several reasons:

- The Federal ethanol program has moved along much more actively and visibly than other government efforts. The accumulating piles of lignin-containing stillage could give a major impetus to research on lignin conversion chemistry;
- The impacts of biomass feedstocks may fall in many more regions of the United States than is the case for shale or coal based feedstocks -- in the forests of the Northwest or Southeast, Midwestern agricultural states, or any major city (although garbage is not as likely a source as the others);
- Use of biomass for feedstocks is in only minor competition with fuel demand (a major exception is the lignin and saccharinic acids burned in paper mills). Rather, much of the proposed biomass would otherwise be used for human or animal food or remain in the fields to maintain soil fertility; and
- Agricultural biomass is a major depository of chemical products (fertilizer, pesticides) and fuel. The chemical cycle could perhaps be integrated; or, at the other extreme, the expenditure of chemicals and fuel may not justify the product obtained.

1.3.6. Summary of Alternative Feedstock Futures

The four scenarios for the year 2000 are summarized here:

- R-2000: Business (or oil) As Usual;
- A-1: Synthesis Gas -- maximum use of coal based syngas and associated by-products;
- A-2: Synfuel By-Products -- use of by-product gases from oil shale and coal liquefaction energy plants; and

- A-3: Biomass -- use of wood processed totally to chemicals, plus some synthesis gas from municipal solid waste.

These scenarios represent MATHTECH estimates of the maximum role that specific feedstocks could play in the chemicals markets. The entry points and market impacts have been identified through careful analysis of feasible Reference Material System pathways for these alternative feedstocks. The use of this formal assessment framework forces the consideration of conversion processes and all related activities required to substitute a new feedstock with attendant environmental problems.

Table 10 shows those chemicals which could become directly available from the alternative sources. That is, the alternative hydrocarbon sources will have new extraction and processing arrangements, but at these points they will mesh into the existing chemical system.

Figures 1 and 2 present the relative distribution of feedstock sources for benzene and ethylene under the four scenarios, as compared to 1980. The other key chemicals in this study are secondary and tertiary chemicals and have more diverse connections to the alternative sources. Thus, they are not amenable to this graphic method.

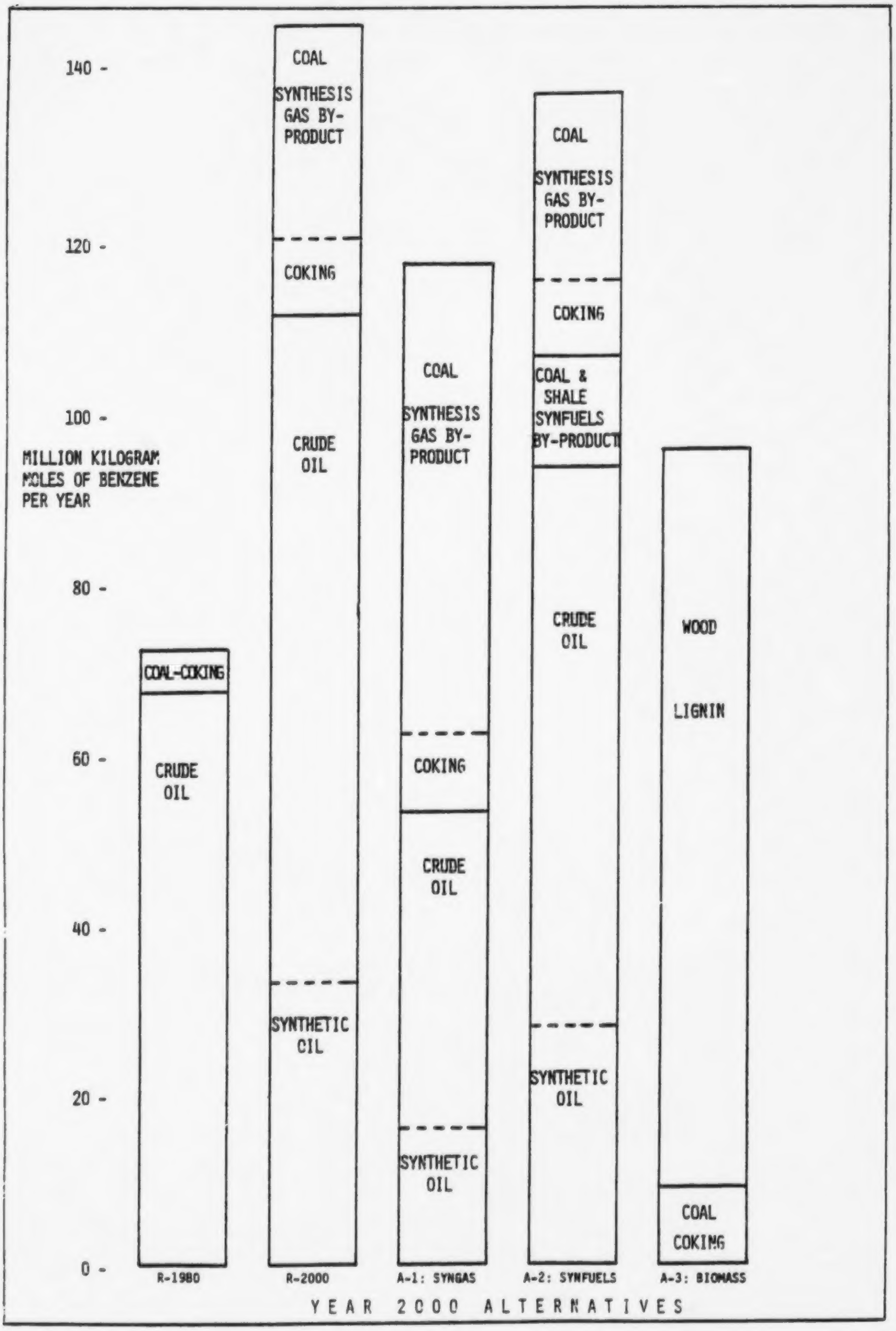
In Figure 1, the increased demand for benzene in R-2000 is supplied both from coal based synthesis gas by-products and from crude oil. In A-1, part of the styrene market for benzene is lost and the synthesis gas by-product supply rises sharply. In A-2, part of the phenol market is taken

Table 10. Summary of Entry Points into Chemical System

Scenario	Sources	Potential Feedstock	Intermediate Chemicals			
			Primary	Secondary	Tertiary	Quarternary
A-1	Coal	Synthesis Gas	ETHYLENE* BENZENE	Ethanol	STYRENE Ethylene Glycol Gasoline	
A-2	Coal Methane Shale Oil	Naphthalene LPG	ETHYLENE BENZENE Propylene Butadiene Xylene Ammonia	Butanol	Phenol Acetone	
A-3	Wood	Cellulose Lignin Synthesis Gas Toluene	ETHYLENE BENZENE Xylene Propylene Butadiene Carbon Black Methanol	CYCLOHEXANE Ethanol Furfural Maleic Anhydride	Acrylic Acid Acetone Leuvlinic Acid Phenol Gasoline	Adhesives HMDA Rubber

*The five principal basic chemicals are shown in capitals.

Figure 1. Benzene Feedstocks Summary



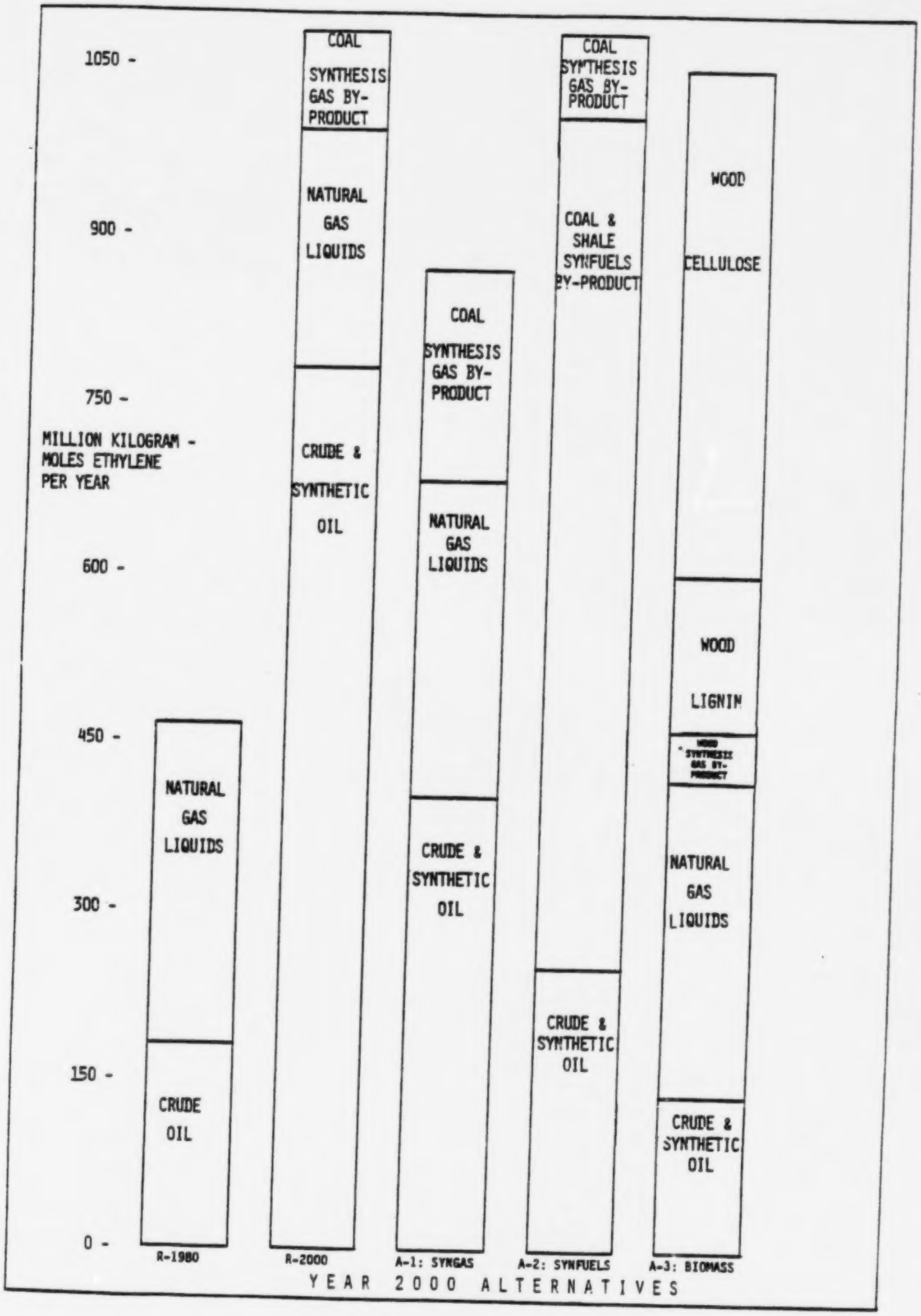
by a synfuel by-product. Finally in A-3, wood lignin based aromatics will saturate the market for benzene (beyond the coal coking supply) and will reduce absolute benzene consumption as well by filling the demand for phenol, cyclohexane, and aniline more directly.

In Figure 2, the R-2000 growth of ethylene is almost entirely from oil, except for some coal synthesis gas by-product. In the synthesis gas scenario (A-1), ethylene loses several markets, especially ethylene glycol, and the demand from oil drops sharply. In A-2, synfuel by-products supply the major part of ethylene demand. In A-3, the ethanol market is lost and nearly half of the remaining ethylene demand is met by dehydrogenating ethanol from fermentation. Additional ethylene would be based on the light hydrocarbons produced during lignin degradation and in combusting residual wood to synthesis gas. With an assumed constant contribution of natural gas liquids, oil would supply less ethylene than in 1980.

Cyclohexane (Chart 3) is most affected in the biomass scenario, A-3. There, both cyclohexane and its competitor in nylon manufacture, phenol, will come from wood processing. Among other nylon chemicals, acrylonitrile may be produced from wood-based propylene and butadiene may be replaced by furfural.

Ethylbenzene (Chart 4) is partially bypassed in styrene manufacture in the synthesis gas scenario, A-1. Toluene is oxidized to benzyl alcohol, which is carbonylated and dehydrated to styrene.

Figure 2. Ethylene Feedstocks Summary



For the chemical industry as a whole, Figure 3 shows the shares of the alternative feedstock sources for each combined Scenario. This comparison utilizes energy units (quadrillion BTUs) rather than the kilogram moles employed elsewhere since there is no better way to aggregate such an array of chemically different feedstocks.* The figure summarizes graphically the source information on Tables 4 and 6 through 7 to compare the overall penetration of the several alternatives under the assumptions used in this report.

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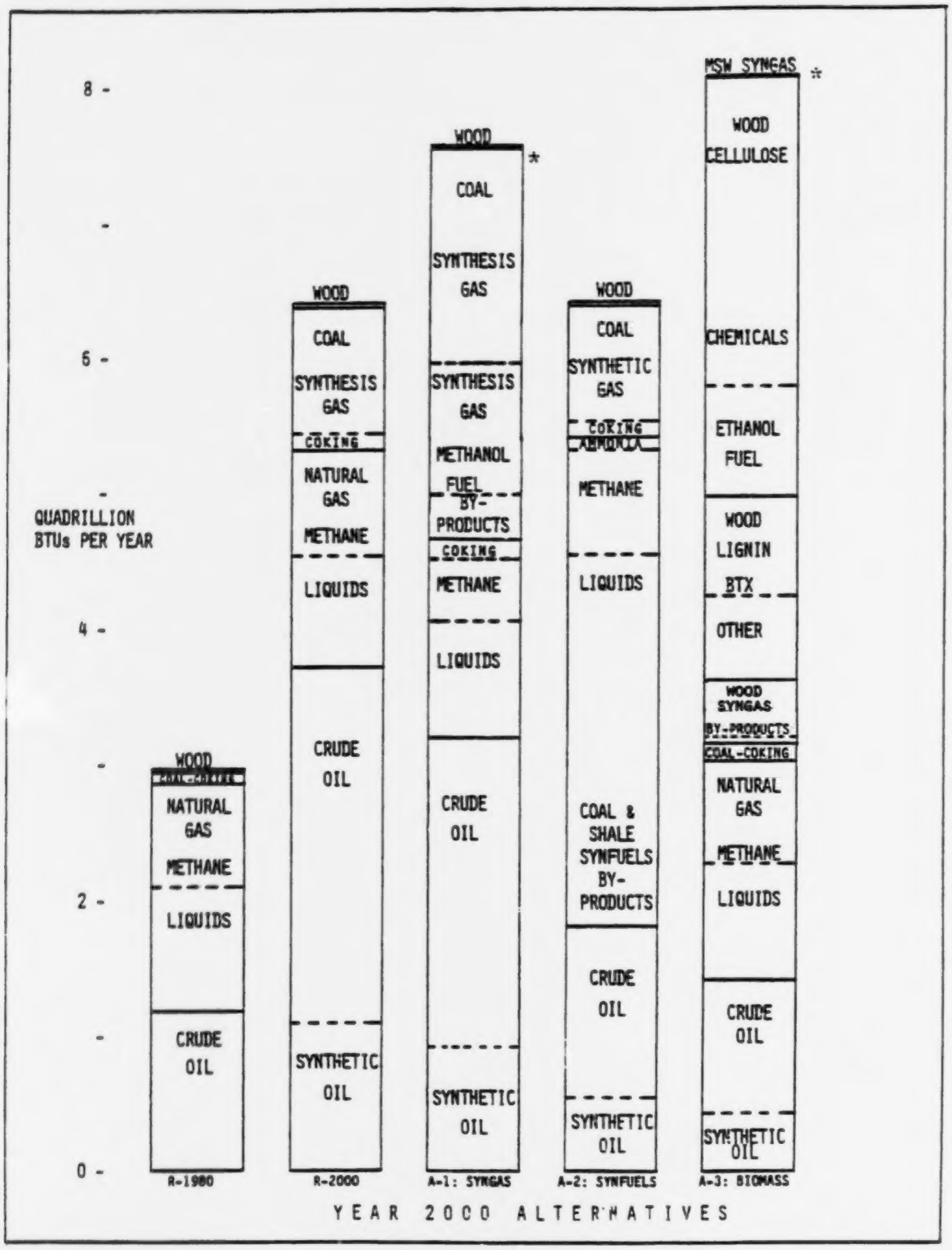
*Problems remain in comparing the shares of various feedstock sources on the basis of their heating values (or as tons of crude oil or coal equivalent). A primary problem in any energy content comparison is that high heating values (HHV) are usually reported, whereas only low heating values (LHV) are achieved in combustion -- the difference is the heat of condensation of the water formed by combustion. Typically that water forms the plume above a smoke stack or is condensed against cooling water, adding to the plant utility load. This discrepancy is greatest for high hydrogen compounds, with methane the extreme case.

A process related problem results from the chemical process industry practice of treating feedstocks and fuel separately. Analytically, how should steam generated in controlling the temperature of a highly exothermic reaction (e.g., methanation) be treated? Similarly, how is the heat generated in a synthesis gas reactor (essentially an oxygen-deficient boiler) recovered and reused? The heat content of coal for synthesis gas is calculated at the plant gate. Since synthesis gas production is exothermic, the feedstock contribution of the coal is exaggerated.

The share of the source is also inflated if a primary conversion step has low conversion to the feedstocks which are of the real interest. For instance, a quarter to a third of coal carbon ends up as carbon dioxide, which is of little value and a possible environmental problem, because of the heat balance and thermodynamics of coal combustion. Similarly, as much as two-thirds of cellulose carbon ends up as CO_2 rather than ethanol in fermentation processes.

Figure 3. Chemical Industry Feedstock Source Summary
(based on energy content)



*The total feedstocks are greater in A-1 and A-3 because the chemical industry is assumed to be supplying additional methanol and ethanol, respectively, as automotive fuels.

In R-2000, the major part of the growth in feedstocks is supplied by crude oil. In A-1, coal other than coking supplies 40 percent of the total feedstocks. In A-2, synfuels by-products could supply as much as 70 percent of total feedstocks. In A-3, biomass supplies 60 percent of all feedstocks.

Note that in scenarios A-1 and A-3, the total chemical industry is expanded by new chemical production of automotive fuels--methanol and ethanol, respectively. Total feedstock demand is further expanded in these two scenarios, out of proportion to demand for chemical products, by the relative inefficiency on a BTU basis of producing synthesis gas from coal and ethanol from wood.

The final summary Table 11 collects and compares on a qualitative scale a variety of characteristics for the possible future scenarios. Comments on some of the technologies involved in these scenarios are presented in Appendix D.

Table 11. Key Characteristics of Alternative Futures

	R-2000 (Baseline)	A-1 (Syngas)	A-2 (Synfuels)	A-3 (Biomass)
Principal Feedstocks	Petroleum Natural Gas	Coal (40%) Petroleum Natural Gas	Synfuel by-products (70%) Petroleum	Biomass (60%) Petroleum Natural Gas
Relation of Growth to Energy Industry	Dependent	Independent	Dependent	Partly Dependent
Initiating Sector	Private	Private	Public	Mixed
Public Awareness	Moderate	Low	Very Low	High - Ethanol Fuel Low - Other
Location	Concentrated	Multi-center	Concentrated	Dispersed
Timing		1990	1990s	2000s
Likelihood	High	High	Moderate to none	Moderate - Ethanol Fuel Low - Other
Key to Technical Development		Catalysts for New Uses	Location; Control of Feed-Rate	Lignin Conversion, Avoiding Distillation, Bioconversion, Process Integration
Greatest Chemical Impact		Ethylene	C_1-C_4	Aromatics

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2. ENVIRONMENTAL IMPACTS: PROBLEM SCOPE AND DEFINITION

This section attempts to define and scope the alternative feedstocks question in terms of its environmental policy and public health implications. It presents forecasts of pertinent environmental values based on the scenarios developed in the previous section and, in conjunction with Appendix E, explains their derivation. Alternative feedstock scenarios are described in terms of underlying environmental and health trends.

2.1. Introduction

The environmental effects of large-scale shifts to alternative chemical feedstocks are evaluated according to the Reference Materials System format. The evaluation proceeds in three discrete steps:

- Assignment of values for residuals and other pertinent quantities to each link in the pertinent RMS trajectories;
- Accumulation of residuals and other quantities on an absolute basis by scenario; and
- Comparison of cumulative values among scenarios and with established benchmarks.

Given the speculative nature of this assignment, however, it is not surprising that many of the RMS trajectories cannot be fully characterized in quantitative terms. A number of technologies, particularly in the biomass area, exist only on paper and have never been examined in environmental terms. Where feasible, such impacts are described qualitatively.

In addition, many important impacts are not of a residual nature. Such things as land use changes and ecological effects are not amenable to summarization in a single figure. Lack of quantification in these cases, however, should by no means be taken to mean a lack of importance. Indeed, the conclusions point out just the opposite -- measures of more conventional pollutants alone do not fully capture the issues of potential environmental importance.

Further, in evaluating the conventional environmental factors, two caveats must be noted. First, residuals are calculated assuming current state-of-the-art control technologies. In instances where substantial impacts are indicated, the development of improved control technology over the coming two decades could mitigate these effects substantially. Second, in instances where impacts appear to be comparatively small on a national basis, local and regional impacts could be large. While it is possible in many cases to project concentrations of residuals on an EPA regional basis, such projections are too coarse to identify problems at the level of the plant site and the surrounding community with any degree of accuracy. These considerations are discussed further in the conclusions of the report, but they should be kept in mind when examining the remainder of this chapter.

One of the basic assumptions made in approaching this study was that feedstock substitution would be viewed entirely as a supply-related phenomenon. That is, demand in the year 2000 is viewed as fixed and feedstocks are supplied to satisfy this demand in a logical and technically consistent manner. As a result of this assumption, incremental environmental impacts are confined almost entirely to the first two RMS sectors, extraction and processing. The following sections will trace the development of the environmental factors scenario-by-scenario on a per unit and cumulative basis, moving "upstream" from processing into the extraction phase.

Another basic assumption further simplifies the assessment process. Simply stated, the operating principle adopted for this study is that environmental impacts will only be attributed to chemicals for those processes which exist primarily for chemical production. Without the motivation and incentive of fuels production, there will be no synfuel-derived feedstocks available to the chemical industry. Thus for the purposes of this report, all environmental impacts in the extraction stage and most in the processing stage of synfuels production are considered a result of the fuels investment decision and cannot logically be assigned to shifts in chemical feedstocks. Specific instances of application of this principle are discussed on a case-by-case basis.

Finally, with regard to data sources for environmental impacts, it should be noted that the technical literature often displays wide variation. The figures chosen represent best technical judgment applied in a conservative manner. In most instances conclusions are relatively insensitive to values chosen. In those instances where the range of values is important, it is discussed with the conclusions.

2.2. Processing Phase

Appendix E establishes sets of environmental coefficients for each trajectory leading to each key chemical in every scenario. Following the RMS format, the derivation of trajectory coefficients was based on the aggregation of coefficients for each process or linkage in the trajectory.

2.2.1. Aggregation of Residuals

With the information derived in Appendix E, total residuals are calculated for each scenario by multiplying the environmental coefficients by the flows associated with each scenario. This is done for each scenario following, with a final section devoted to analyzing the difference among the scenarios and comparing the results to benchmark figures.

(1) *R-1980*. Table 12 details the estimation of residuals associated with the production of the five key chemicals for the current chemical processing system. Table 17 shows the summary aggregation by residual.

It is notable that for the five key chemicals examined in this report, existing processes produce only hydrocarbons as a significant residual. This is a result, basically, of the fact that petrochemicals are a by-product of energy refining processes and that under the operating assumptions of this study, the primary product bears full responsibility

Table 12. R-1980 Aggregated Residuals

Feedstock Source	Chemical Product	Type of Residual	Coefficient	Product Volume Millions of kg/kg mole-yr	=	Total Residual Millions of kg/yr
Oil	Benzene	Hydrocarbons	0.025	67		1.67
	Ethylene	Hydrocarbons	0.015	180		2.7
	Cyclohexane	Hydrocarbons	-	-		-
	Ethylbenzene	Hydrocarbons	0.051	3		0.045
	Styrene	Hydrocarbons	0.042	-		-
Coal Coking	Benzene	Hydrocarbons	0.025	5		0.12

Source: Appendix E

for environmental impact.

(2) R-2000. Table 13 shows the calculation of residuals for the business-as-usual scenario in the year 2000. Residuals for individual trajectories are summed by pollutant in Table 17.

This scenario shows a broader range of residuals because of the inclusion of a relatively modest shift to coal gasification along the lines of current industry plans. The production of each benzene and ethylene from coal contribute equally to these residual totals.

(3) A-1. Residuals for this scenario are calculated in Table 14. The residual summation in Table 17 records an even larger movement to gasification than shown in R-2000. This is reflected in a proportionate increase in residuals across the board. The mix of syngas by-products production does not change. Higher total amounts of residuals in scenario A-1 are still proportional to the amounts given for the R-2000 coal syngas by-products industry.

(4) A-2. Because of the overall assumptions of the study, fewer residuals are generated in this scenario. This is because chemical feedstocks derived from synthetic oil production are treated as by-products and no part of the environmental impact of such production is attributed to chemicals. The calculation of residuals is shown in Table 15.

(5) A-3. Table 16 details the calculation of residuals for this scenario on a trajectory-by-trajectory basis. Table 17 summarizes the results by pollutant.

Table 13. R-2000 Aggregated Residuals

Feedstock Source	Chemical Product	Type of Residual	Coefficient x	Product Volume = Millions of kg/ kg mole-yr	Total Residual Millions of kg/yr
Oil	Benzene	Hydrocarbons	0.025	111	2.8
	Ethylene	Hydrocarbons	0.015	775	11.6
	Cyclohexane	Hydrocarbons	-	-	-
	Ethylbenzene	Hydrocarbons	0.051	8	0.4
	Styrene	Hydrocarbons	0.042	-	-
Coal	Benzene	CO	.13	25	3.2
		NO$_x$	1.9	25	48
		SO$_2$	.9	25	22
		Hydrocarbons	.04	25	1.
		Particulates	.06	25	1.5
		BOD	-	-	-
		Industrial Sludge	16.8	25	420
		Ash	115	25	2900
	Ethylene	CO	.046	85	3.9
		NO$_x$	.92	85	78
		SO$_2$	.348	85	30
		Hydrocarbons	.017	85	1.4
		Particulates	.28	85	24
		BOD	-	-	-
		Industrial Sludge	7.5	85	640
		Ash	51.4	85	4400
Coal Coking	Benzene	Hydrocarbons	0.025	9	0.22

Source: Appendix E

Table 14. A-1 Aggregated Residuals

Feedstock Source	Chemical Product	Type of Residual	Coefficient x	Product Volume = Millions of kg/ kg mole-yr	Total Residual Millions of kg/yr
Oil	Benzene	Hydrocarbons	0.025	53	1.32
	Ethylene	Hydrocarbons	0.015	680	10.2
	Cyclohexane	Hydrocarbons	-	-	-
	Ethylbenzene	Hydrocarbons	0.051	57	2.9
	Styrene	Hydrocarbons	0.042	90	3.8
Coal	Benzene	CO	0.13	55	7.2
		NO_x	1.9	55	104
		SO_2	0.9	55	50
		Hydrocarbons	0.04	55	2.2
		Particulates	0.06	55	3.3
		BOD	-	-	-
		Industrial Sludge	16.8	55	924
		Ash	115	55	6300
	Ethylene	CO	0.046	185	8.5
		NO_x	0.92	185	170
		SO_2	0.348	185	64.4
		Hydrocarbons	0.017	185	3.2
		Particulates	0.28	185	52
		BOD	-	-	-
		Industrial Sludge	7.5	185	1390
		Ash	51.4	185	9510
Coal Coking	Benzene	Hydrocarbons	0.025	9	0.22

Source: Appendix E

Table 15. A-2 Aggregated Residuals

Feedstock Source	Chemical Product	Type of Residual	Coefficient x	Product Volume = Millions of kg/ kg mole-yr	Total Residual Millions of kg/yr
Oil	Benzene	Hydrocarbons	0.025	93	2.3
	Ethylene	Hydrocarbons	0.015	250	3.8
	Cyclohexane	Hydrocarbons	-	-	-
	Ethylbenzene	Hydrocarbons	0.051	8	.41
	Styrene	Hydrocarbons	0.042	-	0
Coal	Benzene	CO	0.13	22	3.0
		NO_x	1.9	22	41,8
		SO_2	0.9	22	20
		Hydrocarbons	0.04	22	1.0
		Particulates	0.06	22	1.3
		BOD	-	-	-
		Industrial Sludge	16.8	22	370
		Ash	115	22	2550
	Ethylene	CO	0.046	75	3.4
		NO_x	0.92	75	69
		SO_2	0.348	75	26.1
		Hydrocarbons	0.017	75	1.3
		Particulates	0.28	75	21
		BOD	-	-	-
		Industrial Sludge	7.5	75	560
		Ash	51.4	75	3860
Coal Coking	Benzene	Hydrocarbons	0.025	9	0.22

Source: Appendix E

Table 16. A-3 Aggregated Residuals

Feedstock Source	Chemical Product	Type of Residual	Coefficient x	Product Volume = Millions of kg/kg mole-yr	Total Residual Millions of kg/yr
Oil	Ethylene	Hydrocarbons	0.015	137	2.06
Coal	Benzene	Hydrocarbons	0.025	9	0.22
Wood/ Cellulose	Ethylene	Hydrocarbons	0.106	450	48
		Particulates	0.006	450	2.7
		BOD	0.57	450	256
		Waste Solids	5.4	450	2430
Wood/ Lignin	Benzene	Particulates	0.018	86	1.55
	Ethylbenzene	Hydrocarbons	.051	85	4.3
	Styrene	Hydrocarbons	.042	90	3.8

Source: Appendix E

Table 17. Summary of Residuals by Scenario

Millions of kg/yr

Scenario	CO	NO_x	SO_2	HYDRO-CARBONS	PARTIC-ULATES	BOD	Secondary Solid Wastes: Noncombustible and Sludge
R-1980	-	-	-	4	-	-	-
R-2000	8	143	61	17	26	-	9,488
A-1	17	292	122	26	52	-	19,337
A-2	7	75	128	11	23	-	8,503
A-3	-	-	-	48	4	256	2,430

The biomass scenario gives a much different mix of residuals than do the other coal-related scenarios. The particular emphasis here is on water pollutants, especially biological oxygen demand. The particular trajectory of major importance involves the production of ethylene from cellulose.

(6) Comparative Analysis. Table 18 attempts to place the alternative feedstocks question in perspective with regard to national estimates.

Since the important policy questions involve the potential changes that can occur by 2000, this table shows increments above 1980 for each scenario. The last line of the table shows increments (or decrements) by residual on a national basis as estimated elsewhere by EPA.*

On a national basis, there appears to be only two points of concern; one is associated with the biomass scenario A-3. Only a small increment in biological oxygen demand is expected nationally. This increment, however, could be raised by over 50 percent from the processing of wood to chemicals, particularly to ethylene.

Another concern could possibly arise with regard to hydrocarbon emissions. There is little increase projected nationally for hydrocarbons; however, if the A-3 biomass scenario replaces

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*Taken from EPA, Environmental Outlook, 1980. Since this report does not include a 1980 baseline, increments were calculated from 1985 figures. The use of a 1985 baseline is not believed to affect any conclusions drawn from it. An average of 1975 and 1985 figures produced no significant differences.

Table 18. Change from 1980 Baseline

Millions of kg/yr

	CO	NO_x	SO_2	HYDROCARBONS	PARTICULATES	BOD	Secondary Solid Wastes: Noncombustibles and Sludge
R-2000	8	143	61	17	26	-	9,488
A- 1	17	292	122	26	52	-	19,342
A- 2	7	75	128	11	23	-	8,503
A- 3	-	-	-	48	4	256	2,430
National Increment: * All Sources, net emissions	8979	4535	4535	91	3174	454	123,779

*Derived from Environmental Outlook 1980. The increments are calculated from 1985 rather than 1980 and, thus, underestimate the actual 1980 increment.

the R-2000 chemical portion of the EPA projection, the national hydrocarbon increment would rise by a third.

2.2.2. Regional Distribution

While, in most instances, analysis of residuals from alternative chemical feedstocks indicates little cause for concern at an overall, national level, the same is not necessarily true at the regional or local level. Chemical processing operations currently take place in almost every state, but they are highly concentrated in terms of volume (and, thus, in terms of environmental impact) in only a few key areas. Significant movements to alternative feedstocks, as depicted in the different scenarios discussed above, have the potential for redistributing processing activity geographically, thereby altering the pattern of regional environmental impact.

(1) R-1980. Geographical location of basic and intermediate chemical processing capacity is approximately distributed by EPA region as shown in Table 19 (23).

Concentration of basic and intermediate chemical capacity in Region VI is currently such as to make the contribution of any other region insignificant. Of the Region VI total, 77 percent of the relevant capacity is located on the Texas Gulf Coast and 23 percent is located on the Louisiana Gulf Coast.

(2) R-2000. The business-as-usual scenario as envisioned in R-2000 includes a rather modest syngas development, mainly in Regions III, IV, V, VI, and VIII. While this development

Table 19. Distribution of Basic Chemical Processing Capacity

Percentage by EPA Region

Region	States	R-1980*	R-2000	A-1	A-2	A-3
I	CT, ME, MA, NH, RI, VT	0	0	0	0	2
II	NJ, NY, PR, VI	9	8	5	3	5
III	DE, DC, MD, PA WV, VA	3	5	8	4	3
IV	AL, FL, GA, KY, MS, NC, SC, TN	2	4	7	4	47
V	IL, IN, MI, MN, OH, WN	5	6	9	2	5
VI	AR, LA, NM OK, TX	79	68	54	24	33
VII	IA, KA, MO, NE	1	1	1	0	1
VIII	CO, MT, ND, SD, UT, WY	0	6	16	63	1
IX	AZ, CA, HA, NV	1	1	1	0	1
X	AK, ID, WA, OR	0	0	0	0	2

*Extrapolated from the locations of installed capacity for ethylene and benzene, as shown in Directory of Chemical Producers, 1980, SRI International, Menlo Park CA.

Totals may not add to 100 due to rounding.

is small in an energy context, it is significant in terms of chemical feedstocks and results in these regions (other than VI) acquiring an additional 11 percent of basic and intermediate chemical capacity in 2000 (assuming that processing capacity locates at the source of feedstocks).

Although the Region VI share (Table 19) of chemical capacity drops from 79 percent to 68 percent, the absolute size of the Gulf Coast industry still increases by two-thirds.

The magnitudes of residuals resulting from the R-2000 changes are in every instance insignificant.

(3) A-1. Synthesis gas as a source of chemical feedstocks would come from coal. Coal for gasification would probably originate either in the Appalachian area, in the Midwest, or in the Mountain and Great Plains states. The presence of a gasification plant, however, does not necessarily indicate the co-location of processing facilities. While grassroots mine-mouth chemical plants might be attractive in some instances, transportation of synthetic natural gas by pipeline to existing processing plants (on the Gulf) might in some instances appear better. Detailed exploration and analysis of such decisions is beyond the scope of this paper, but it is possible to examine the potential for geographical redistribution in a more judgmental fashion.

One approach is to examine announced gasification plans to try to determine the locational pattern. Using plans for U.S. methanol plants relying on government financing (28) as a starting point and modifying the list to include pure gasification facilities, privately-financed projects, etc. (3,29), it is possible to distribute plants by probable regional location of coal sources. In approximate terms, the distribution appears as follows:

Region III	15%
IV	15%
V	15%
VI	15%
VIII	40%

Using this rough geographical pattern and assuming mine mouth location, the distribution of basic chemical production capacity can be determined.

According to A-1, 39 percent of chemical feedstocks are derived from coal gasification in 2000. If the remainder is assumed to be distributed in the same manner as in R-1980 and if coal use is assumed to be divided among the Western, Midwestern, and Appalachian states as shown above, the regional percentage distribution will appear as shown in Table 19, if all syngas processing takes place at mine mouth.

This redistribution implies a basic chemical processing industry nearly as large in absolute terms as that existing in Texas today, emerging in the states of Colorado, Montana, North Dakota, South Dakota, Utah and Wyoming.

In terms of processing residuals, the only measurable impact appears to be on NO_x emissions in Region VIII. In comparison to the EPA low growth NO_x scenario for Region VIII, a movement to synthesis gas, as shown in A-1, could potentially increase NO_x emissions by six percent.

(4) A-2. The synfuel by-products scenario suggests an even more massive shift of chemical activity to the Western states (assuming that product is not piped to existing chemical plants). Again, it is doubtful that economics and natural limitations, particularly water, will permit such a massive transformation of the industry in a relatively short time period. However, as an extreme example the pattern of distribution is of interest.

In A-2, 56 percent of by-product chemical feedstocks originate in shale, coal, and tar sands, primarily located in the Western states. This results in the distribution shown in Table 19. Under such conditions, Region VIII absorbs 63 percent of basic chemical processing in 2000, while Region VI falls to 24 percent.

From the standpoint of residuals generation, however, there is little relative impact, either positively for Region VIII or negatively for Region VI. This is because (1) the fuels portion of the synfuel industry dwarfs the chemicals portion and (2) the remaining petroleum and gas fuels industry in Region VI totally overshadows any lost chemicals activity.

In terms of indirect environmental effects, however, the relative impact on Region VIII could be larger. Currently, 166,000 persons are employed in the basic organic chemicals industry (24). If employment is assumed to grow only half as rapidly as the physical output of industry (as productivity increases), 250,000 persons will be employed in 2000. Further, assuming that employment is located in direct proportion to production, 58,000 jobs would be created in Region VIII over the next 20 years. If each job means a population increment of four persons (25), the chemical industry would promote the migration of over 630,000 persons to Region VIII under this scenario. This would represent an increase of nearly ten percent over EPA's low growth baseline of seven million population (26). Such a population increase would of and by itself create a significant number of jobs secondarily related to chemicals together with a significant range of environmental impacts.

(5) A-3. The biomass scenario depicts a massive shift to wood and other renewables as the source of chemical feedstocks. In this case, the logistics of material extraction make more certain the location of chemical processing facilities at the material source. Processing plants would probably be smaller in scale, less concentrated, and located in rural areas, close to the sources of biomass.

However, since biomass is produced in every region, it is more difficult to determine where chemical capacity will locate. Today, the pulp and paper industry is located (Table 20) largely in Regions IV and V (Southeast and Great Lakes), indicating two possible regions of interest for chemicals from biomass (26). Considerable tree harvesting also takes place in the Region X (Northwest) for the production of lumber, plywood and particle board.

Regional preferences for chemical biomass production will depend primarily upon the economics of the extraction phase,

Table 20: Output of the Pulp and Paper Industry, By EPA Region: 1975 and 2000

		1975		2000	
	Region	Output ($ Millions)[a]	Percent of Total	Output ($ Millions)[a]	Percent of Total
I.	New England	$ 2,510	14	$ 4,960	11
II.	New York/New Jersey	1,660	9	2,800	6
III.	Middle Atlantic	1,577	9	3,475	7
IV.	Southeast	3,758	20	11,915	25
V.	Great Lakes	5,247	28	12,396	26
VI.	South Central	1,337	7	4,656	10
VII.	Central	363	2	1,009	2
VIII.	Mountain	53	-	249	1
IX.	West	662	4	1,976	4
X.	Northwest	1,379	7	3,579	8
	Total	$18,530	100	$47,015	100

[a] Constant 1971 dollars.

Source: USEPA. Environmental Outlook, EPA 600/8-80-003, U.S. Environmental Protection Agency, Office of Research and Development, Washington, D.C., 1980.

rather than of the processing phase, and this will be discussed further in the subsequent section. For purposes of this evaluation, however, it is assumed that biomass for chemicals will originate principally from the intensive cultivation of trees in the Southeast (Region IV), based on the attractive climate, terrain, and location of this Region with respect to chemical consumers. Seventy-five percent of biomass productivity is arbitrarily assigned to Region IV, with the remainder assumed uniformly distributed across the remaining Regions. Tree farming for the explicit purpose of chemicals production is assumed only to occur in Region IV.

Under this assumption, geographical distribution appears as shown in Table 19. Region IV becomes the nation's chemical center under A-3, and Region VI is reduced to five-sixths of its current size in terms of chemical capacity.

This massive shift is associated with at least one potentially serious environmental consequence. As pointed out previously, the fermentation process in the wood-to-ethylene trajectory generates large increments of biological oxygen demand when the residue is discharged to receiving waters after being treated to current standards. This process alone could increase Region IV BOD emissions in 2000 by over 50 percent. This phenomenon, however, is almost certainly treatable and, therefore, avoidable.

Probably of more concern would be the potential socioeconomic impacts of locating biomass chemical plants in rural regions of the Southeast. Wood chemical plants would be a combination of activities now found both at pulp and paper and at chemical plants, and Scenario A-3 would require around 86 such plants, based on efficient plant capacities of two billion kilograms of wood per year, a figure based in turn on existing capacities of pulp and paper plants.

While no figures can be found authoritatively estimating the labor requirements of such a plant, operations would clearly be labor intensive, particularly if batch chemical processing were relied upon. A very rough estimate of employment is 2500 persons per plant (24). This then totals to 234,000 overall in order to satisfy the A-3 scenario. This is a large number and clearly poses some potential for environmental impact in rural areas, even though it represents a very small proportion of the total employment in Region IV in the year 2000.

2.3. Resource Extraction Phase

Resource extraction is a general term, referring in the RMS format to that phase in the production of a chemical where the starting materials are separated from nature and transported to processing. From the RMS standpoint, each resource has a trajectory including extraction, preparation, and transportation taking it to the point of initial processing.

Several simplifying assumptions make assessment of this phase less complex than that of the processing stage; however, a lack of hard data at the same time makes the assessment much more qualitative. The assumptions are:

- Since chemicals from synfuel refining are considered to be by-products, the extraction phase for Scenario A-2 is not meaningful; and
- Although extraction and transportation of oil and gas have well-known environmental impacts, they are not assessed here because there will be little variation from these sources among scenarios.

The remaining resource extractions of interest are coal for gasification and wood for biomass. These will be examined in terms of Scenarios A-1 and A-3 only, where those resources are emphasized.

It should be noted that while environmental effects were considered in the processing stage only for the five key chemicals, they are considered here for the scenario as a whole. As a reference point, the five key chemicals represent about half of the chemical activity in each scenario.

2.3.1. Scenario A-1

The coal gasification scenario affects the environment in numerous ways during extraction. Synthesis gas based chemical plants will vary in size according to (1) the size of the available coal source, ideally a local mine with a 20 year supply, and (2) the size and location of the market for the products, varying, for instance, from 27 million kg moles of ethanol or the small, location-specific market for cellulose acetate film up to 1150 million kg moles of methanol, much of which could be absorbed by the fuel market in the refinery-poor Great Plains. The plants may be expected to range from about 300,000 tons of coal per year, typical for the eventual TVA ammonia plant or the Eastman Chemicals plant under construction, up to ten million tons per year, as might be used in the proposed North Dakota lignite-to-methanol plant (28). For comparison, synthetic natural gas plants fall in the upper part of this range, around five million tons. At a median size of three million tons of coal per year, which could support a plant making half a dozen important derivative chemicals, the A-1 scenario would involve about 47 such "coal-plexes," requiring approximately 140 million tons of coal per year (taking the higher heat content of Eastern coal into account).

To put this quantity in perspective, the total coal mined in the United States in 1980 was 825 million tons. EPA projects this amount to increase to 1660 million tons (26) in 2000, whereas DOE has forecast production of as much as 2000 million tons (1). Thus, chemical feedstocks in 2000 under Scenario A-1 would require an amount of coal equivalent to around 17 percent of 1980 production and only seven or eight percent of estimated production in the year 2000.

Coal for gasification will come from the West and Midwest and from the Appalachian area. East of the Mississippi, coal potentially can be extracted from both deep and surface mines. Scenario A-1 envisions, however, that coal for Eastern gasification plants will be supplied in the year 2000 mainly from underground mines. This assumption rests on the fact that surface mining in the Appalachian region and in the Midwest is already on the decline, currently accounting for less than 50 percent of Eastern production (1). Environmental regulation has made such mining very expensive in the East at the same time that Western coal fields are beginning to open. Also, it appears that technological advances in underground mining, such as longwall techniques, have the potential for greatly increasing productivity and for improving safety conditions. The Department of Energy foresees surface mining producing less than a fifth of Eastern coal in 2000 (1).

(1) Eastern coal extraction. Coal production from east of the Mississippi (Regions III, IV, and V) is estimated by the Energy Department to be around 950 million tons in 2000 (1). If 30 percent of the A-1 coal gasification activity takes place in Regions III and IV, 36 million tons of high quality Eastern coal will be required. This will represent around seven percent of the Appalachian total. If, as assumed, 15 percent of coal gasification activity takes place in Region V (the Midwest), there will be a five percent increment to the regional coal production forecast for 2000.

Underground mines produce negligible air emissions, but coal preparation and cleaning does produce pollutants. The environmental coefficients and total residuals produced according to the assumptions of A-1 are shown in Table 21. Figures for total dissolved and suspended solids and for solid waste generation applicable to both Regions III and IV are also shown.

Table 21. Residuals from Underground Mining and Coal Cleaning

	Southern Appalachian Mining			Northern Appalachian Mining			Illinois Basin Mining			Coal Cleaning (per region)			
	TDS	TSS	Solid Waste	TDS	TSS	Solid Waste	TDS	TSS	Solid Waste	Dust	NO_x	SO_x	Solid Waste
Coefficient (lb/ton of mined coal)	7.7	.1	120	18.8	.3	562	8.3	.14	39	.4	.17	6.7	1120
Residual Quantity* (thousand tons)	69	.9	1080	169	2.7	5058	75	1.2	351	3.6	15.3	60	10080

*assumes that 15 percent of national production for chemical feedstocks occurs in Southern Appalachia (Region IV), 15 percent occurs in Northern Appalachia (Region III) and 15 percent in the Illinois Basin (Region V). Total Eastern coal production is 54 million tons per year.

Source: The Aerospace Corporation. Energy Technologies and the Environment. Environmental Information Handbook. DOE/EV/74010-1, U.S. Dept. of Energy, 1980.

In most cases the hypothetical residuals appear insignificant on a regional basis. There is one exception: total dissolved solids (TDS) appear to comprise around eight percent of the Region III total for 2000 (26). Solid waste generation also appears significant, but a direct comparison with regional figures is difficult.

In addition to the impacts documented above, acid drainage from underground mines can represent a severe environmental problem where the coal is rich in sulfide impurities. Such impurities can be oxidized to sulfuric acid and the resulting lower pH of groundwater increases the solubility of toxic heavy metal compounds such as arsenic and cadmium. The acidity and heavy metals may damage aquatic life and make water unfit for human use. Acid drainage is particularly a problem from abandoned or unattended mines and, thus, will not appear in full measure until considerably after the year 2000 scenario date. The major region of impact for acid drainage is Region III, which is projected to account for roughly one-half of all sulfate discharges nationally in 1985 (1, 26).

The impacts of underground mining on land use are direct and site specific. Although less conspicuous than the results of surface mining, subsidence from underground mines can have severe impacts on roads, water and gas lines, buildings, and local hydrology. The extent, severity, and timing of subsidence depend on overburden composition and thickness, mining technique, and other factors. It has been estimated that approximately 25 percent of the eight million acres* of undermined lands in the Eastern United States have subsided (1). Because of the complex nature and uncertainty of subsidence, land use impacts on adjacent lands may increase the area affected by a factor of five (1). The area affected by underground mining is thus greater than that affected by surface mines with the same production capacity. Subsidence can occur during the operating phase of a mine. However, with certain mining techniques (e.g., room-and-pillar mining), it is more likely to occur many years later as pillars collapse. Each year's production of 54 million tons of Eastern and Midwestern coal could at some future time potentially disturb over 11,000 acres, roughly a ten percent share of all subsidence potentially attributable to underground coal mining in 2000 (1).

Underground coal mining is two to three times more labor intensive than is surface mining (24); even so, the employment increment due to coal mining in support of chemicals production is likely to be relatively minor. Depending on the future level of labor productivity, production of 54 million tons per year of underground coal will probably require between 12,000 and 26,000 workers. If current levels of productivity are maintained, 26,000 individuals will join 216,000 already employed in underground mining east of the Mississippi in 2000. This is a significant increment for the industry, but it will probably not generate environmental impacts by causing migration to rural areas. Rural Appalachia particularly is burdened with high unemployment and can probably alone absorb such an increase without undue stress. For contrast, combined employment in Regions III, IV, and V in 2000 is expected to be around 55 million.

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*An acre is equivalent to 4047 square meters.

(2) Western coal extraction. Coal production from the West (Regions VI and VIII) is estimated by DOE to be about 1000 million tons in 2000 (1). If 55 percent of the A-1 coal gasification activity takes place in these regions as assumed, 86 million tons per year of lower quality Western coal and lignite will be required. This represents around eight percent of the Western total. According to the assumptions stated earlier, 75 percent of Western coal would originate in Region VIII.

In contrast to Eastern underground mining, Western surface mining is more notable in terms of air pollutants produced, while at the same time producing few water pollutants. Water pollution is not a problem principally because of the aridity of the region. Low rainfall minimizes runoff, and low groundwater tables minimize the risks of leaching. Also, the natural alkalinity of Western formations make the acid drainage problem negligible in any case (31).

Water supply and availability is of particular concern to coal production in the West. Although water requirements for mining are negligible compared to other end uses and water for coal preparation is continually recycled, competition for limited water supplies in uses such as energy transportation (e.g., coal slurry pipelines) could become a major constraint on development of alternative chemical feedstocks.

Potential sources of airborne emissions from surface mining activities include dust and other materials emitted during the blasting and materials handling operations, major combustion products released by the diesel oil-fueled equipment used in mining operations, and wind-blown dust from mines and waste piles. In some surface mining operations, waste piles ignite spontaneously and burn, releasing products of combustion and other, unburned materials into the atmosphere. Residuals are calculated and summarized in Table 22.

A potentially more important source of emissions is the coal preparation process. Raw coal must be crushed and washed by various methods to remove impurities. It is then dewatered and thermally dried. Convection driers produce the air emissions of concern here (31). Coefficients and residuals for these processes are shown in Table 22. Comparison with projections of Region VIII air emissions shows significant emissions of NO_x and hydrocarbons from the preparation stage. In each case, the combined emissions associated with coal mining, preparation and processing can increase projected Region VIII emissions by more than a third, assuming that regional distribution patterns approximate those derived here.

Increases in surface mining in the West will substantially affect land use. However, because of significantly thicker seams, mining of Western coal reserves will affect fewer acres per ton of coal than mining elsewhere in the country (31).

Table 22. Residuals from Western Surface Mining and Coal Preparation

	Mining (1)					Preparation (2)					
	Dust	SO_x	NO_x	CO	HC	Dust	SO_x	NO_x	CO	HC	Solid Waste
Coefficient (lb/ton of mined coal)	1.2	0.006	0.07	0.02	0.006	0 .2	0 .9	9	2.6	3.4	571
Residual Quantity* (thousand tons)	52	0 .3	3.0	0 .9	0 .3	8.6	39	387	111.8	146.2	24,550

*Based on 86 million tons per year of coal

Sources: (1) White, I.L. et al. Energy from the West: Energy Resource Development Systems Report Volume II: Coal. PB-299-178. U.S. Environmental Protection Agency, Office of Energy, Minerals, and Industry, Washington, DC, March 1979.

(2) The Aerospace Corporation, Energy Technologies and the Environment. Environmental Information Handbook. DOE/EV/74010-1. U.S. Dept. of Energy, 1980.

The most obvious impact of surface mining is the temporary removal of land from its use as farmland, forest, or rangeland. Spoil from improperly controlled mines can result in erosion and landslides, and unreclaimed highwalls are a major esthetic problem. Noise, visual, and hydrologic impacts beyond the mine boundary affect wildlife habitats and recreational activities in a larger area. Experience in most coal-producing regions suggests that once the coal has been extracted, the land can be successfully reclaimed to support its former uses. However, in some of the more ecologically fragile areas, particularly arid Western lands, experience is inadequate to ensure successful reclamation (31).

The A-1 scenario suggests that somewhere on the order of 3500 acres will be disturbed annually by Western surface mining in order to produce chemical feedstocks (1). This compares with estimates of 40,000 acres per year disturbance as a result of all coal production on Western lands -- less than ten percent of the total (1).

Since Western coal mines are extremely capital intensive, labor requirements for operations are quite small. The 86 million ton requirement for the West assumed in Scenario A-1 would probably involve only 4-5000 workers -- as compared to three to five times more for Eastern underground mining (24). While this is an insignificant number on a regional basis, extremely rural communities can become "boom towns" with influxes of far fewer workers. The socioeconomic impacts of such "boom towns" have been widely recognized and subjected to exhaustive study (25).

2.3.2. Scenario A-3

The biomass scenario is partially a result of major assumptions about the U.S. fuels program. It is assumed that the current objectives of the Federal ethanol production program -- 11-12 billion gallons* per year by 1990 -- are met. The primary biomass source for this program is corn, but it is widely believed that corn can provide only seven to eight billion gallons of the total objective. In terms of today's conversion technologies, the remaining four billion gallons of ethanol would almost certainly be derived from wood.

Ethanol production will utilize only half of total wood inputs, leaving enormous amounts of lignin as a by-product. This lignin is almost certain to be utilized in some manner, providing impetus for the development of lignin conversion chemistry. Once the chemical industry begins to utilize chemical feedstocks from wood, the scenario envisions rapid expansion beyond the limits of the ethanol program.

Scenario A-3 in the year 2000 will require 250 million tons of wood. This is equivalent to the total harvesting of the forest products industry in 1980 for all uses (paper, lumber, etc.) (24). The question that must be first addressed with regard to this volume is: How will it be produced? There is a range of potential alternatives for producing wood of this amount. First of all, it should be noted that in the United States approximately 1000 million tons of woody biomass are grown each year (33) and a similar amount is removed from the ecosystem. As mentioned, one quarter of this is taken for pulp and paper and solid wood; the remaining three-quarters succumbs through natural causes -- disease, insects, wildlife, fire and wind -- and is oxidized back into the carbon cycle (10). It is theoretically conceivable that woody biomass could be harvested for chemical purposes without overly damaging this balance, since, unlike paper or lumber processing, chemical production processes can accept a large variety of trees, both in terms of species and size. If economical, fallen, damaged and diseased trees could conceivably fill the demand.

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*A gallon is equivalent to 0.003785 cubic meters.

Tree harvesting for the pulp and paper industry is quite selective since the processes in use are designed for high fiber content. These are characteristics of larger, more mature trees. For chemical feedstock purposes, however, trees can be very small and immature. This means, first, that timber can be raised much like an agricultural crop, using the faster-growing hardwood varities that are not desirable for paper, and harvesting with automated machinery rather than with chain saws.

These characteristics suggest that chemical feedstocks would push the forest products industry strongly in the direction of silviculture or tree "farming." Silviculture (as the term is used in this report) can be distinguished from current commercial practices by a lack of selectivity in harvesting, intensive use of fertilizer, pesticides and fungicides, and very rapid growth cycles (26).

Silviculture can raise the productivity of forest land greatly. While yields vary greatly with region, type of tree, etc., the current average for forest lands is two to three tons/acre/year. Silviculture would raise this to around ten tons/acre/year, primarily by reducing growing time from 30-40 to ten years (10). At such a yield, the chemical industry envisioned in A-3 would require 25 million acres in order to be self-sustaining, an acreage equivalent to only five percent of U.S. land currently classified as commercial timberland, but an area roughly the size of Kentucky.

The environmental impacts associated with silviculture are very similar to those of agriculture in general. At present, a number of environmental problems confront U.S. agriculture, ranging from water pollution to topsoil loss. Intensive agriculture, as practiced in most areas of the United States, is highly dependent on chemical fertilizers and pesticides, on water availability, and on fossil-fuel inputs. The practice of intensive tree farming would suffer from similar limitations. Heavy fertilization, large-scale irrigation, chemical control of pests, and the use of machinery could all result in additional pollution and environmental degradation.

In the case of forest residues, environmental effects are important, since removal of residues could lower the level of organic matter in the soil, and increase nutrient removal. However, most of the residues can usually be removed without significant harm and, indeed, positive environmental impacts of forest-residue removal have been postulated, including reduced frequency and intensity of forest fires and the alleviation of residue buildup in streams (11). However, the amount of disturbance necessary to remove these scattered residues may cause increased erosion and fugitive dust. In addition, the reduction in forest residue may increase erosion, leading to losses of valuable topsoil and to increased sediment in streams. Increased biomass removal will also increase water removal from soil.

An important question in the possible establishment of tree farms is their impact on wildlife habitats, migratory pathways, and endangered species. If large areas presently considered marginal for agriculture or forestry are planted to biomass crops, the effects on wildlife could be significant because of habitat reduction or change, particularly if a tree monoculture replaces a species-rich habitat. On the other hand, while wildlife is obviously disturbed in the harvested area, modern harvesting practice allows movement of animals into the wooded environs. Also, a regenerating, vigorously growing young forest can be a better habitat for wildlife, supporting larger populations than a mature forest that does not provide sufficient shelter and food (10).

Silviculture would clearly contribute to non-point source water pollution, but the actual magnitude of the effect is not certain. The most important non-point source pollutant nationwide is sediment, and on a per acre basis sediment loss from recently cut timberland is 2.5 times that from cropland (26). However, the basis of silviculture lies in rapidly growing trees and rapid growth reduces the exposure time of deforested land. Of the 25 million acres potentially devoted to biomass farming in A-3, only 2.5 would be clear-cut in any given year. If vulnerability to erosion lasts for two years, five million acres would be exposed on an annual basis. Using the 2.5 factor, this is equivalent to adding 12.5 million acres to agriculture. Such an area represents less than six percent of the land expected to be under cultivation in 2000 (26), and thus the national sediment impact should be quite small. This is also true in Region IV (Southeast) where gross sediment discharges will represent around 30 percent of the national total for agriculture in 2000 (26).

However, while rapid growth may minimize sediment problems, much of the rapidity is gained through the use of fertilizers. Although there is no clear agreement on the extent of soil depletion associated with silviculture or on the fertilizer applications necessary, one source quotes figures that place the fertilizer needs of treelands at around two-thirds those of average cropland (5). These figures are shown in Table 23.

Table 23. Comparative Fertilizer Inputs (lbs/acre)

Nutrient	Silviculture*	Illinois Corn
Nitrogen	107	148
Phosphorus	14	41
Potassium	54	79
Total	175	268

*Based on 25 percent fertilizer efficiency.

Sources: (1) Argonne National Laboratory. Environmental and Economic Evaluation of Energy Recovery from Agricultural and Forestry Residues. DOE/EV-0106 VC-58b, U.S. Dept of Energy, Office of Environmental Assessment, Washington, DC 1980.

(2) Society of American Foresters. Proceedings of the Tenth Annual Spring Symposium for the Florida Section. Energy from Forestry, Production and Use. 1978.

Using the 25 million acres figure arrived at earlier, total nutrient usage for silviculture in Scenario A-3 amounts to around 2.2 million tons, broken down as indicated in Table 23. Since only 500,000 acres of commercial forest lands currently receive fertilizer applications in any year (5,26), this represents a large increase. Compared to total estimated nutrient runoff, however, the increment appears much smaller. Average national runoff appears to be 40 percent of application (26) (this may be less for forest lands due to the sheltering effect of the leaf cover) and applying this factor to the nutrient total estimate for silviculture gives 880,000 tons as the projection for nutrient runoff. This is between six and seven percent of total gross nutrient discharges estimated for agriculture in 2000 (26).

If, however, silviculture for chemicals is 75 percent concentrated in Region IV, as can be postulated on the basis of climate and location, the increase appears more severe. Specifically, nutrient runoff is estimated at 2,760,000 tons in 2000, up by 77 percent from 1980 (26). The additional runoff from silviculture could add 25 percent to the 2000 total.

Another environmental problem of interest in this scenario is that of pesticide use. Toxic insecticides, fungicides, herbicides and rodenticides used to protect forests may be deposited directly in surface water by careless application, or be transported in surface runoff. Currently almost no pesticides are applied to commercial forests and little is known about what types might be necessary for silviculture or in what amounts. Nationally, discharges of pesticides to surface waters are expected to increase dramatically in the next twenty years, and any additional contribution from silviculture is potentially hazardous (5).

Solid waste from silviculture is not expected to present problems, since almost all forest products can be used in the chemicals process.

There are no specific estimates of employment necessary to support a tree farm, but rough approximations can be made using current forestry practices. While the actual harvesting of a tree farm might be much more mechanized than is current harvesting practice, there will be considerable labor needed for crop maintenance, fertilization, pest control, etc., much as is needed in any intensive agricultural operation. Each plant requires around 200,000 acres of land to be self-sustaining (10); thus, labor requirements are relatively high. It appears that perhaps 1,000 workers will be necessary for the tree farming component of each wood chemicals plant (24). Overall, this amounts to 125,000 for Scenario A-3. In combination with the chemical processing component, this brings the estimate of total potential employment to approximately 359,000 for this scenario. Again, while this amounts to less than two percent of expected employment in Region IV in 2000 (24), its rural nature must be a strong source of environmental concern.

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3. CONCLUSIONS AND RECOMMENDATIONS

3.1. Introduction

This section attempts to identify major information/ knowledge gaps in our ability to assess the potential for alternative chemical feedstocks, and to identify actions on the part of the Federal government that could affect the course of events in a constructive manner. It describes the degree of confidence and certainty in data, methods and findings and identifies research in this area which might be conducted to support the Agency's regulation mission.

Prior to this, however, it is important to review the overall intent and conduct of the study and the manner in which conclusions and recommendations should be viewed.

3.1.1. Restatement of Objectives

A Mini-Assessment differs considerably from more conventional technological impact studies. Some of the points of differentiation are the following:

- The Mini-Assessment is speculative and future oriented rather than definitive. It is intended to depart, when necessary, from firmly based scientific data and to substitute judgmental factors as appropriate;

- The Mini-Assessmment, by its nature, deals with highly uncertain futures and, thus, must express its conclusions in terms of probabilities;
- The Mini-Assessment is aimed as much at discovering areas of deficient information as at applying existing information to particular problems; and
- The Mini-Assessment is short in duration and employs the minimal resources to survey an extensive topic. The objective is breadth, rather than depth in coverage.

In light of these points, it should be emphasized that the scenarios derived in this study do not represent forecasts, but the limits of possible directions of change for the chemical industry.

It is quite conceivable that all of the major alternative feedstocks identified -- coal-derived synthesis gas, synfuel by-products, and biomass -- could simultaneously be in use in the year 2000. The share of total feedstock demand for each new source would consequently fall short of the individual scenario impacts.

The ultimate objective of this Mini-Assessment, then, is not to direct EPA's attention to a particular forecasted future, but to "raise the consciousness" of the regulators with regard to the important effects of different futures and to point out the events that might move industry in each direction.

3.1.2. The Probablity/Impact Interface

Conclusions in a study of this type have no usefulness unless associated with a probability of occurrence. Probabilities, of course, are highly speculative, but their use is certainly within the "ground rules" of the Mini-Assessment concept. Problems occur in assessments of this sort, however, when layers of conditional probablities occur. Take, for instance, the probability that water pollution will occur in EPA Region III as a result of synthesis gas production. To calculate such a probability (p), the following algorithm must be followed:

> p (synthesis gas scenario) X p (production in Appalachia) X p (coal from underground mining) X p (production in Region III) X p (control levels) X p (significance of discharge)

Obviously, this results in the multiplication of many small numbers, which will, of course, produce a much smaller number. Comparison of such small and uncertain numbers does not appear to be productive. Instead, in cases of this sort, probabilities are presented in rank order form rather than in absolute terms. Absolute probabilities are employed only for the higher level, unconditional events. However expressed, all probabilities represent only professional judgment.

3.2. Overall Assessment of Environmental Impacts

3.2.1. Key Environmental Issues

In very general terms, the environmental concerns identified in this study can be summarized as follows:

- o For synthesis gas from coal, air pollution in the West, water pollution in the East;

- For synfuel by-products, socioeconomic impacts in the West; and
- For wood biomass, water pollution and socioeconomic impacts in the East

More specifically, the ten most prominent impacts identified in the study are listed in Table 24. The order of listing is by MATHTECH judgment of potential severity and each impact is associated with the EPA Region most likely to be affected.

(1) Severity Ranking. Four of the top ten items are associated with Scenario A-3 (wood biomass), five with Scenario A-1 (coal gasification) and one with Scenario A-2 (synfuels). Biomass tends to dominate the top of the list, coal gasification the bottom. The synfuels route to chemicals is inherently low in environmental impact because of the by-product nature of the chemical feedstocks.

In regional terms, Region IV is affected by five of these potential problems (both from A-1 and A-3), while Regions III and VIII are each noted three times. It should be pointed out that the regional distribution was determined largely by assumption and is highly speculative.

The biomass scenario (A-3) assumes the most intensive activity takes place in the Southeast (Region IV), due to its inherent attractiveness to wood farming in terms of rainfall, terrain, growing season, access to markets and established forest products industry, and assumes some form of large scale

Table 24. Ten Prominent Environmental Concerns

(listed in relative order of severity)

Problem	Region Likely Affected	Scenario
1. Nutrient and pesticide runoff	IV (Southeast)	A-3
2. BOD discharges	IV	A-3
3. Socioeconomic impacts	VIII (Mountain)	A-2
4. Socioeconomic impacts	IV	A-3
5. Hydrocarbon emissions	VIII	A-1
6. NO_x emissions	VIII	A-1
7. Total dissolved solids discharge	III (Middle Atlantic)	A-1
8. Land subsidence	III, IV and V (Great Lakes)	A-1
9. Acid drainage	III	A-1
10. Disturbance of wildlife habitats	IV	A-3

silviculture. The wood farming phase of activity will produce very large loadings of nutrients in ground and surface waters, smaller loadings of sediment, and unknown but certainly significant loadings of pesticides. In the processing phase, the production of ethylene from cellulose creates large amounts of biological oxygen demand. This is thought to be potentially less severe than the non-point source discharges because it is more capable of being controlled.

Combined wood plantations and chemical processing complexes will be located by definition in rural areas and will directly employ perhaps 3500 people each. Such an operation has significant potential for socioeconomic disruption and the environmental problems often associated with rapid population growth in undeveloped areas. Disruption of wildlife habitats is a potential problem, but less severe than the others. To the extent that silviculture is not employed, impacts will be less severe.

The coal gasification scenario (A-1) is divided almost evenly between the Western states (Regions VI and VIII) and the Eastern states (Regions III, IV, and V). The Eastern half of the activity is divided evenly among Regions III, IV, and V, while 75 percent of Western activity takes place in Region VIII. Such a division is basically a result of observation of the locations now specifically planned for synthesis gas plants. They are split in rough terms along such lines.

It is further assumed that Eastern syngas will be produced from coal from underground mines, due to continued tight regulation of Appalachian and Midwestern surface mining. This assumption leads to potential problems of acid drainage and total dissolved solids (TDS) particularly in the Northern Appalachian area (Region III), and land subsidence in all regions.

The pristine nature of Region VIII makes it sensitive to particulate emissions form coal preparation operations and the overall gasification process. NO_x emissions similarly have the potential to affect this region.

Scenario A-2 assumes all environmental effects would be associated with chemical plants located in conjunction with synfuels facilities. The by-product nature of the chemical operations limits the environmental effects, but the labor-intensiveness of the chemical industry relative to petroleum refining makes the chemicals component significant in terms of employment. The potential socioeconomic impacts of chemical-induced population shifts are quite large for Region VIII.

(2) Likelihood ranking. Severity must be considered in the context of likelihood. The ten items discussed above have been reordered in terms of likelihood and a rank order matrix is shown in Figure 4. This matrix allows a comparison of the joint severity/likelihood of each listed impact. Generally speaking, those falling in the upper left-hand quadrant are

Figure 4. Severity/Likelihood Rank Order Matrix

LESSER LIKELIHOOD →

LESSER SEVERITY ↓

	1. Hydrocarbon emissions (VIII)	2. NO$_x$ emissions (VIII)	3. TDS discharge (III)	4. Socioeconomic impacts (VIII)	5. Nutrient and Pesticide runoff (IV)	6. Acid drainage (III)	7. Socioeconomic impacts (IV)	8. BOD discharges (IV)	9. Land subsidence (III, IV, & V)	10. Disturbance of wildlife habitats (IV)
1. Nutrient and pesticide runoff (IV)					✓					
2. BOD discharges (IV)								✓		
3. Socioeconomic impacts (VIII)				✓						
4. Socioeconomic impacts (IV)							✓			
5. Hydrocarbon emissions (VIII)									✓	
6. NO$_x$ emissions (VIII)		✓								
7. TDS discharge (III)	✓								✓	
8. Land subsidence (III, IV, & V)			✓							
9. Acid drainage (III)						✓				
10. Disturbance of wildlife habitats (IV)										✓

more important than are those in the lower right-hand quadrant. The other two quadrants have mixed values.

Three impact items unambiguously appear to be more important than the others:

- Nutrient and pesticide runoff (Region IV);
- Socioeconomic impacts (Region VIII); and
- Hydrocarbon emissions (Region VIII).

Two others also appear to be of a similar order of importance:

- NO_x emissions (Region VIII); and
- Total dissolved solids discharges (Region III).

The likelihood ranking is primarily affected by the likelihood of the overall scenario. Coal gasification is thought to be most likely; synfuels development less so; and biomass to chemicals least likely. Acid drainage and subsidence problems are given lower rankings than their scenario would indicate because their major effects will probably occur after the year 2000, even though activity prior to that time will be responsible for the occurrence.

3.2.2. Information Deficiencies

One of objectives of a Mini-Assessment is to point out pertinent areas in which information deficiencies occur. Ten of the more important areas are shown in Table 25. It is not at all surprising that the wood-to-chemicals scenario dominates the list. This is clearly the area about which least is known, from the basic chemistry through the socioeconomic impacts.

Table 25. Ten Important Areas of Information Deficiency

Scenario A-1

1. Geographical/economic factors affecting syngas locational decisions
2. Generation of trace elements and toxic substances in effluents

Scenario A-2

3. Geographical/economic factors affecting by-product chemical locational decisions

Scenario A-3

4. Pesticide needs of silviculture
5. Geographical/economic factors affecting biomass chemical locational decisions
6. Lignin chemistry and processing technology
7. Design factors for representative wood plantation/chemical processing plant
8. Competitive economics vis-a-vis other chemical feedstocks
9. Ecological effects of silviculture
10. Technological aspects of controlling silviculture runoff

The one item that carries through the three scenarios relates to the geographical and economic factors that affect choice of location for chemical processing and related activities. Since it is clear that the environmental impacts of alternative chemical feedstocks will be almost entirely regional and local in nature, it is critical to develop better information on the potential locational patterns for each scenario. This study has been conducted using crude judgmental factors and gross assumptions regarding location.

3.3. Initiating Events

An important aspect of a Mini-Assessment is the assembly of information on the decision process that leads to the scenarios of interest. This accomplishes two purposes: first, it provides EPA with a means of tracking progress toward or away from any particular scenario. Second, it provides a disciplined approach for assessing the probability of occurence for any scenario.

3.3.1. The Futurescan Process

In order to place all Mini-Assessments on a common basis for evaluation, OER has adapted a standard format for assessing initiating events based on the Futurescan model (a model developed for OER by the Futures Group). The logic of the format begins with consideration of the historical time series for quantities pertinent to the Mini-Assessment. Each time series is then projected into the future using standard statistical procedures embodied in the Futurescan model.

It is at this point that the evaluation process begins. For each series of interest, a list of "events" is identified. An event is defined as any verifiable and independent impact on the historical trend of the time series quantity. "Verifiable" and "independent" mean that the impact occurs at a point in time and is not directly related to historical trends. An example might be a breakthrough in technology leading to a much cheaper product or higher labor productivity.

For each event cataloged, a cumulative probability of occurrence is postulated for specified years in the future. While the probability assigned to each event is the result of professional judgment alone, it is believed that focusing on the initiating events allows a much better overall assessment of scenario probabilities than does focusing on the overall scenario.

In addition to probabilities, impact information is required. First, years to first impact must be specified. In other words, given that the initiating event occurs, how long will it take for the time series to be affected in a discernible manner. Subsequently, two additional similar quantities must be judged: years to maximum impact and years to steady state impact. The thought here is that oscillations in impact might be expected; impact might go from zero to some high value before returning to a more permanent and predictable, but lower, value.

Finally, the extent of both the maximum and steady state impacts must be estimated. These are calculated in terms of percentages of the time series quantity as projected in the years in which maximum and steady state impacts might occur. Again, all such quantities are judgmental in nature, but the focus on underlying causes allows a scenario to be evaluated in a consistent and verifiable manner.

3.3.2. Events and Sequences

Tables 26 through 28 lay out the initiating events and their probabilities and magnitudes for the three commodity time series that are basic to this study. The commodities are coal, both Western and Eastern, and wood from the Southeastern region. It was not possible to utilize measures more closely correlated to alternative chemical feedstocks, such as synthesis gas and synthetic fuels, since historical time series are either nonexistent or meaningless. Note that in all cases, steady state and maximum impacts are equivalent.

For both Western and Eastern coal, the list of initiating events is the same, as are probabilities and years to impact. Impacts, however, differ, since they are stated as percentages of different base quantities and since the effect of some events is to redistribute activity between Eastern and Western regions. This can be seen most clearly in the case of Event Number 5, where reduced Eastern mining productivity acts to shift coal production to the West, creating a substantial impact on Western coal and leaving the East at its historical trend line.

Table 26. Eastern Coal (Regions III, IV and V) Scenario: A-1

EVENT NO.	POTENTIALLY IMPORTANT EVENTS	PROBABILITY			YEARS TO FIRST IMPACT	YEARS TO MAX. IMPACT	MAX. IMPACT (%)	YEARS TO STEADY STATE IMPACT	STEADY STATE IMPACT (%)
		1985	1990	2000					
1	Large scale deployment of methanol as a gasoline additive (10%) through government committment	0	.4	.8	6.0	20.0	350	20.0	350
2	Successful scale-up of chemical synthesis via coal products to maximize penetration in chemical markets	.5	.9	.95	2.0	20.0	180	20.0	180
3	Relative price increase (25%) in price of oil and gas	.1	.3	.6	4.0	12.0	1000	12.0	1000
4	Natural gas rationing gives low priority to chemicals (50% decline)	0	.2	.4	2.0	10.0	320	10.0	320
5	Reduced relative productivity in Eastern coal	.1	.3	.5	1.0	10.0	0.0	10.0	0.0
6	More permissive coal leasing and regulatory policies	.8	.8	.8	1.0	10.0	470	10.0	470

Table 27. Western Coal (Regions VI and VIII) Scenario: A-1

EVENT NO.	POTENTIALLY IMPORTANT EVENTS	PROBABILITY			YEARS TO FIRST IMPACT	YEARS TO MAX. IMPACT	MAX. IMPACT (%)	YEARS TO STEADY STATE IMPACT	STEADY STATE IMPACT (%)
		1985	1990	2000					
1	Large scale deployment of methanol as a gasoline additive (10%) through government committment	0	.4	.8	6.0	20.0	250	20.0	250
2	Successful scale-up of chemical synthesis via coal products to maximize penetration in chemical markets	.5	.9	.95	2.0	20.0	130	20.0	130
3	Relative price increase (25%) in price of oil and gas	.1	.3	.6	4.0	12.0	110	12.0	110
4	Natural gas rationing gives low priority to chemicals (50% decline)	0	.2	.4	2.0	10.0	330	10.0	330
5	Reduced relative productivity in Eastern coal	.1	.3	.5	1.0	10.0	170	10.0	170
6	More permissive coal leasing and regulatory policies	.8	.8	.8	1.0	10.0	140	10.0	140

Table 28 . Wood Products (Region IV) Scenario A-3

EVENT NO.	POTENTIALLY IMPORTANT EVENTS	PROBABILITY			YEARS TO FIRST IMPACT	YEARS TO MAX. IMPACT	MAX. IMPACT (%)	YEARS TO STEADY STATE IMPACT	STEADY STATE IMPACT (%)
		1985	1990	2000					
1	Large scale deployment of ethanol as gasoline additive (10%) through government committment	0	.2	.3	6.0	20.0	120	20.0	120
2	Breakthrough on lignin chemistry to open aromatics market	0	.1	.2	15.0	25.0	325	25.0	325
3	Breakthrough in ethanol technology to make competitive with other products	.2	.4	.6	4.0	15.0	300	15.0	300
4	Significant increase in relative price of coal (25%)	0	.1	.2	6.0	20.0	400	20.0	400
5	More restrictive regulation on coal and other fossil fuels	0	.2	.2	10.0	20.0	175	20.0	175
6	More permissive policies toward forest lands	.8	.8	.8	10.0	20.0	100	20.0	100

Overall, the greatest inducement toward the synthesis gas scenario is seen to be a significant increase in the price of oil and gas with respect to coal. While such an event also produces a fairly rapid impact, the probabilities associated with it are quite low. Several other events possess high probabilities -- Federal methanol program, successful scale-up of coal to chemical technologies, and more permissive regulation of coal mining and leasing of coal properties -- but lower overall impacts. (The regulatory event aids Western coal at the expense of the East.)

In the case of the biomass scenario, lower probabilities, generally speaking, are associated with higher impacts. Here again, price is seen as the major initiating force in terms of impact. It also operates fairly rapidly, but the probability of a significant change in the price of coal with respect to wood is considered to be very low. Another important event is the state of ethanol production technology. A breakthrough in fermentation technology could intensify the government's commitment to ethanol development and stimulate research and development in the area of lignin technology.

In summary, while coal gasification is primarily driven by economic forces, wood chemicals will be affected by both economic and technological developments.

3.4. Recommendations

Recommendations following the foregoing analysis and conclusions fall into two categories: (1) those events that should be tracked in the interest of predicting the substitution of alternative chemical feedstocks, and (2) research projects worthy of consideration in addressing the potential problems associated with alternative feedstocks.

3.4.1. Key Events

In general, two types of events should be of interest in tracking and forecasting the use of alternative feedstocks. One type is the low probability, high impact event; the other is the low impact event that can lead to a sequence of other events with high cumulative impact.

The prime example of the first type of event is a rapid and significant change in the relative price structure among coal, wood, and oil and gas. A major change in these relationships would be a clear precursor in changes in the likelihood of alternative feedstocks use.

The major event of the second type is the technology for converting wood to ethanol. Were a breakthrough to occur in the fermentation process technology, Federal support for the ethanol fuel program could increase, giving subsequent impetus to the development of lignin chemistry. Looking at this another way, perhaps the best route for inducing the growth of the wood-to-chemicals industry would be to encourage the development of new ethanol fermentation technology.

3.4.2. Research Recommendations

One of the purposes of this Mini-Assessment is to provide a basis for the planning and evaluation of the research and development program being carried out in EPA. R&D is long term by nature and it is essential for doing the best possible job in anticipating future problems and research needs. The results of this Mini-Assessment do indicate several areas where R&D might contribute to better understanding of potential damage pathways and controls related to the use of alternative feedstocks. It must be pointed out, however, that the scope of this study did not include a thorough review of current research and development activities. Thus, we cannot judge whether or not the current program is responsive to these needs. The objective in this section _is_, therefore, to identify the major issues that may be dealt with through research and development. It is _not_ to evaluate the current research plan or to develop a revised plan. The R&D recommendations are discussed as they apply to the major divisions organized under EPA's Office of Research and Development.

(1) _Monitoring and Technical Support._ Potential changes in feedstock patterns will lead to new sites and regional locations for chemical plants, such as those that will locate near coal liquefaction, ethanol and other synthetic fuel plants. Although the environmental effects of chemical operations will not be more serious or extensive than those now encountered in such regions as the Gulf Coast, the shift in location poses

monitoring problems. Methods and instrumentation must be available to give timely information in regions where the sensitivity to chemical spills, emissions, etc., will generally be greater. Personnel must be trained in the use of monitoring equipment and the interpretation of analytical results. It is recommended that, as these new sites are identified, or become apparent, surveys be made of the adaptability of monitoring equipment to the sites and of the availability of personnel trained or trainable in the use and interpretation of monitoring equipment.

(2) Environmental Engineering and Technology. A number of new processes involving the large scale handling of solid and waste materials (coal and biomass) have been identified. The effort devoted to engineering of environmental controls for these processes as energy conversion systems is quite large. There has, however, been little effort devoted to controls for chemical processes that may be coupled to these energy facilities. The assessment of ongoing research relevant to this problem was beyond the scope of this study. It is recommended that R&D programs be evaluated for relevance to this problem including the following high priority areas:

- Control of potentially large BOD problems associated with biomass conversion;
- Disposal of chemical and solid wastes at plant sites;
- Technical characterization of representative combined silviculture/chemical processing facilities; and

- Assessment of geographical/ economic factors affecting the locational decisions of chemical firms.

(3) Environmental Processes and Effects Research. The release of wastes and emissions from chemical plants in new locations poses several research problems associated with environmental processes and research. Attention should be given to the relevance of the R&D program to the following issues:

- Natural processes involving BOD from biomass conversion and effects in the region of the plant including local streams, lakes etc.;
- Processes and effects involving pesticides associated with biomass conversions;
- Toxic materials involved in coal conversion processes; and
- Ecological effects of silviculture.

(4) Health Research. A number of problems related to the BOD, pesticide, and waste problems discussed previously arise in the understanding of damage functions and other health effects. These involve both direct effects and indirect effects occurring through air, water, or the food chain. Potential damage pathways should be identified for specific plants and processes as the basis for evaluation of the relevance of ongoing health research to these problems associated with alternative feedstocks.

APPENDIX A. THE REFERENCE MATERIALS SYSTEM

The chemical feedstock system involves a complex series of chemical conversions and processes producing a wide variety of final products. The selection of specific feedstocks to produce these chemicals is heavily dependent on the relative cost and availability of the feedstock as well as on the industrial infrastructure that exists in the chemical industry. Transition to new feedstocks that are often located in different regions of the country, or abroad, take a considerable amount of time. Several substitution patterns, related to chemical byproducts from synthetic fuels, biomass, and the improved economics of synthesis gas produced from coal, do appear to be inevitable in the long run. There remain, however, a large number of uncertainties regarding timing, technologies, economics, and environmental effects that must be monitored on a continuous or periodic basis.

At the start of the Mini-Assessment of alternative feedstocks it was apparent that there would be a large number of gaps in the information base and considerable uncertainty in several key areas. For that reason, the proposal included the development and use of an integrating framework -- the Reference Materials System -- that could serve both to organize the information developed in the Mini-Assessment and to provide an ongoing capability for the addition of future information gleaned from follow-on assessments and monitoring of technical progress in alternative feedstocks. The application of the Reference Materials System to this Mini-Assessment has been described earlier in the report. This Appendix provides an overview of the potential of the Reference Materials System as a general framework for the integration of information on materials intensive processes and industries where environmental problems may be anticipated.

The Reference Materials System was developed by Hoffman and Bhagat while at Brookhaven National Laboratory in order to evaluate and assess renewable sources of materials and compare them with nonrenewable sources on an equivalent basis with standardized assumptions and definitions. This work was done initially for the Committee on Renewable Resources for Industrial Materials (CORRIM) of the National Academy of Sciences.

The Reference Materials System (RMS) is a network description of the flow of material resources from resource extraction through refinement, production, and transportation processes to the utilization, maintenance, and recycling operations. It thus links alternative resources and feedstocks to specific markets through pathways involving the processing and conversion steps with attendant environmental problems. The system may be employed to assess material production technologies and to evaluate substitution possibilities. It is most appropriate for representing the process steps and infrastructure to apply alternative resources as feedstocks for the production of basic chemicals. Problems related to public health, public welfare, and environmental policy arise potentially at each step in the production cycle including resource recovery, transportation, conversion, and the production of the basic chemicals. The objective of the Mini-Assessment was to define in sufficient depth the specific problems that could arise in order to help EPA develop research priorities and allocate EPA resources to address those problems. Network diagrams were developed for the five basic chemicals selected for detailed analysis and for other chemicals, such as synthesis gas, that were felt to be important intermediaries in future changes in feedstock patterns. The Reference Material System was defined for these chemicals for the base year, 1980, and projected to a future year, 2000, for each scenario.

In the course of the Mini-Assessment, deficiencies in the information base were identified. These deficiencies included:

- Inconsistent data on processes;
- Incomplete data and gaps; and
- Incomplete and inconsistent forecasts.

Many of these inconsistencies arise from the style and scope of past studies where attention was focused on particular chemicals or sectors without regard for alternatives and other sectors that might affect the sector of interest. As an example, studies of synthetic fuels have concentrated on energy products with little attention paid to possible chemical by-products. Use of a consistent format, such as the Reference Materials System, across all of the sectors quickly uncovers gaps and inconsistencies.

Problems of scope arise even in this Mini-Assessment, where the reality of overseas competition for feedstocks and chemicals was not addressed directly. Our intent was to identify environmental problems arising in the United States assuming that domestic feedstocks remained viable, whether as a result of national policy or economics. A more complete and detailed assessment should characterize the economics of overseas sources such the Persian Gulf.

In summary, the experience gained in this Mini-Assessment has demonstrated the need for and utility of a comprehensive information framework such as the Reference Materials System. This system served the following critical roles:

1. Provided a framework to integrate data on the
    - o Resource base;
    - o Processes and conversion;
    - o Infrastructure; and
    - o Market demand.

2. Provided a compact representation of scenarios in a standard format sufficiently simple to be prepared in handbook form or computerized.

3. Presented a format that facilitates analysis of impacts of changes in market share, technologies, and the resource base.

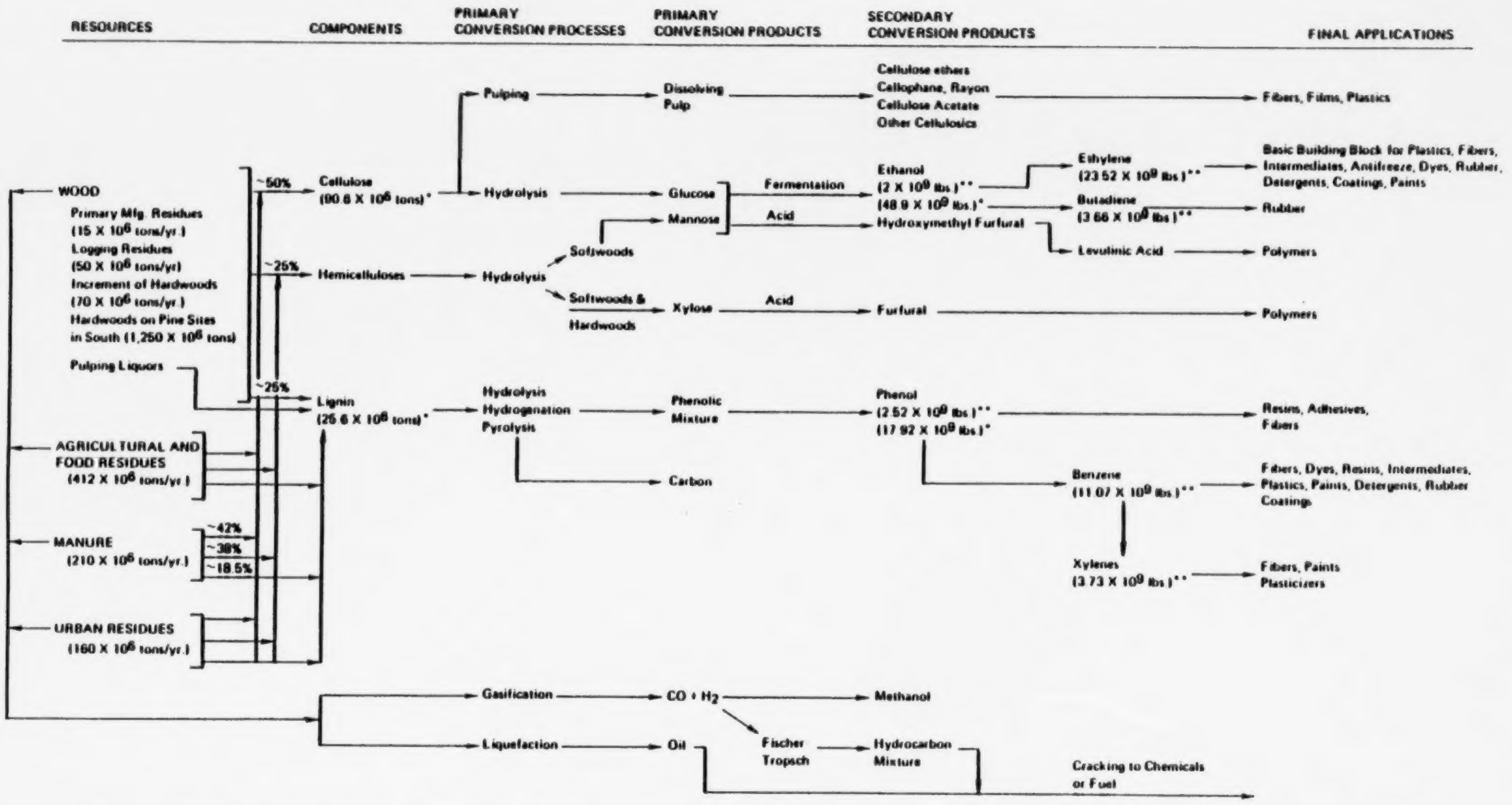
The RMS provides a framework for integrating engineering and economic information on alternative resources and conversion processes into a comprehensive systems framework. The network flow diagram can be quantified in terms of the mass flow of all renewable and nonrenewable materials on an annual basis through each step of the system corresponding to a given scenario. A variety of data elements including capital and labor requirements may be organized in this framework along with environmental impacts and issues that arise at various steps in the system. This process description of the energy and materials system has also been coupled with economic policy models of the input-output or econometric variety to ensure proper analysis of the role of energy and materials in the overall economy. The fact that the assessment framework is compatible with these analytical approaches is important to any future use of the system by EPA-OSASS.

The Reference Materials System concept has been employed, as indicated previously, as the central systems analysis approach by the Committee on Renewable Resources for Industrial Materials (CORRIM) of the National Research and Development (R&D) programs needed to overcome the barriers to production and use of renewable resources. The RMS approach has also been adopted for a study in Ireland concerned with the use of biomass as a source of energy and feedstocks. The use of renewable resources as a source of industrial feedstocks and chemicals was addressed in the CORRIM study, and the simplified network prepared for that study is presented in Figure A.1.

A comprehensive RMS -- involving a network representation of the flow of all materials for 1977 from the resource side, through all of the "activities" listed along the top, to a specific end use such as building and construction -- is shown in Figure A.2. This figure is quantified in terms of the mass of material flowing annually through each activity. The material flows on the supply side were obtained from the Statistical Abstract and from the annual statistical reports put out by various trade associations; the data on the demand side were estimated using the product mixes and conversion ratios, as they existed in the year 1974, from the CORRIM Materials Source Book. The network can also be quantified in terms of energy use, cost, labor, and environmental effects associated with each activity. A path from a specific resource to a specific end use is called a "trajectory." Each "activity" in the trajectory represents a technical process or production step that is characterized by both a material flow element (and material losses) and the relevant data elements, e.g., energy requirements, other material inputs, labor and capital needs, and environmental effects. Imports and exports of resources and products can be indicated by flow vectors from and into the appropriate nodes.

The RMS feedstock subsystems described elsewhere in this report and the associated data may be employed to analyze the

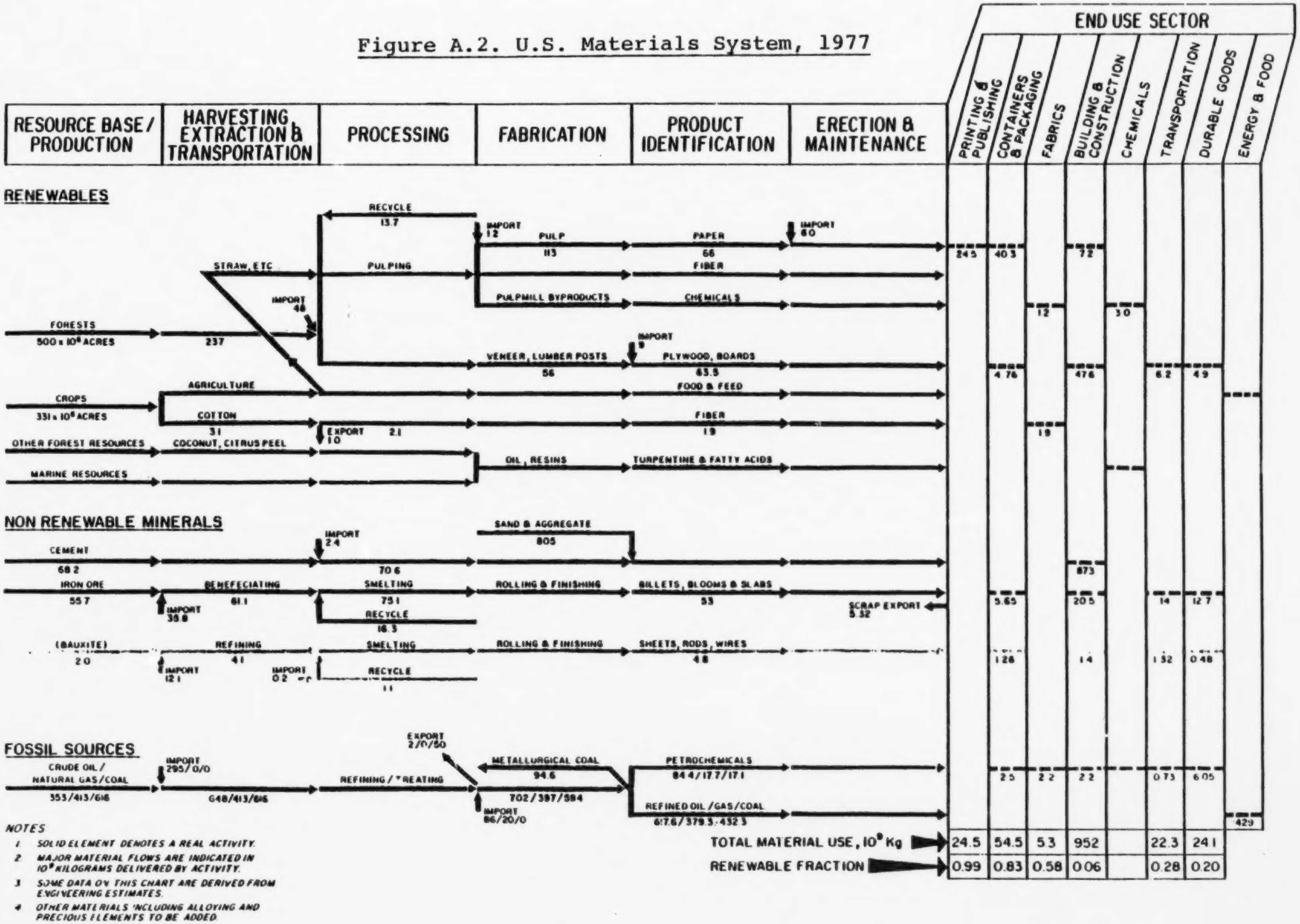
Figure A.1. Future Potential Flow of Wood and Agricultural, Municipal and Feedlot Residues for Chemical Use


RESOURCES
COMPONENTS
PRIMARY CONVERSION PROCESSES
PRIMARY CONVERSION PRODUCTS
SECONDARY CONVERSION PRODUCTS
FINAL APPLICATIONS
WOOD
Primary Mfg. Residues (15 X 10⁶ tons/yr.)
Logging Residues (50 X 10⁶ tons/yr)
Increment of Hardwoods (70 X 10⁶ tons/yr.)
Hardwoods on Pine Sites in South (1,250 X 10⁶ tons)
Pulping Liquors
AGRICULTURAL AND FOOD RESIDUES (412 X 10⁶ tons/yr.)
MANURE (210 X 10⁶ tons/yr.)
URBAN RESIDUES (160 X 10⁶ tons/yr.)
~50%
~25%
~25%
~42%
~38%
~18.5%
Cellulose (90.6 X 10⁶ tons)*
Hemicelluloses
Lignin (25.6 X 10⁶ tons)*
Pulping
Hydrolysis
Hydrolysis
Softwoods
Softwoods & Hardwoods
Hydrolysis
Hydrogenation
Pyrolysis
Gasification
Liquefaction
Dissolving Pulp
Glucose
Mannose
Xylose
Phenolic Mixture
Carbon
CO + H2
Oil
Fermentation
Acid
Acid
Fischer Tropsch
Cellulose ethers
Cellophane, Rayon
Cellulose Acetate
Other Cellulosics
Ethanol (2 X 10⁹ lbs.)** (48.9 X 10⁹ lbs.)*
Hydroxymethyl Furfural
Furfural
Phenol (2.52 X 10⁹ lbs.)** (17.92 X 10⁹ lbs.)*
Methanol
Hydrocarbon Mixture
Ethylene (23.52 X 10⁹ lbs.)**
Butadiene (3.66 X 10⁹ lbs.)**
Levulinic Acid
Benzene (11.07 X 10⁹ lbs.)**
Xylenes (3.73 X 10⁹ lbs.)**
Cracking to Chemicals or Fuel
Fibers, Films, Plastics
Basic Building Block for Plastics, Fibers, Intermediates, Antifreeze, Dyes, Rubber, Detergents, Coatings, Paints
Rubber
Polymers
Polymers
Resins, Adhesives, Fibers
Fibers, Dyes, Resins, Intermediates, Plastics, Paints, Detergents, Rubber Coatings
Fibers, Paints Plasticizers

*Quantity needed for 1974 production of Benzene, Butadiene, Ethanol, Ethylene, Phenol and Xylenes. Cellulose quantity may include Hemicelluloses yielding mannose.

**1974 production (Ethanol and Phenol derived from Ethylene and Benzene instead of vice versa). (Xylenes not derived from Benzene)

Figure A.2. U.S. Materials System, 1977


RESOURCE BASE / PRODUCTION
HARVESTING EXTRACTION & TRANSPORTATION
PROCESSING
FABRICATION
PRODUCT IDENTIFICATION
ERECTION & MAINTENANCE
END USE SECTOR
PRINTING & PUBLISHING
CONTAINERS & PACKAGING
FABRICS
BUILDING & CONSTRUCTION
CHEMICALS
TRANSPORTATION
DURABLE GOODS
ENERGY & FOOD
RENEWABLES
FORESTS
500 x 10⁶ ACRES
237
STRAW, ETC
IMPORT 48
RECYCLE 13.7
PULPING
IMPORT 12
PULP 113
PAPER 66
IMPORT 60
FIBER
PULPMILL BYPRODUCTS
CHEMICALS
VENEER, LUMBER POSTS 56
IMPORT 9
PLYWOOD, BOARDS 63.5
CROPS
331 x 10⁶ ACRES
AGRICULTURE
FOOD & FEED
COTTON 31
EXPORT 10
21
FIBER 19
OTHER FOREST RESOURCES
COCONUT, CITRUS PEEL
MARINE RESOURCES
OIL, RESINS
TURPENTINE & FATTY ACIDS
NON RENEWABLE MINERALS
CEMENT 68.2
IMPORT 2.4
70.6
SAND & AGGREGATE 805
IRON ORE 55.7
IMPORT 30.8
BENEFECIATING 61.1
SMELTING 75.1
RECYCLE 16.3
ROLLING & FINISHING
BILLETS, BLOOMS & SLABS 53
SCRAP EXPORT 5.32
(BAUXITE) 2.0
IMPORT 12.1
REFINING 4.1
IMPORT 0.2
SMELTING
RECYCLE 1.1
ROLLING & FINISHING
SHEETS, RODS, WIRES 4.8
FOSSIL SOURCES
CRUDE OIL / NATURAL GAS/COAL
353/413/616
IMPORT 295/0/0
648/413/616
REFINING / TREATING
EXPORT 2/0/50
IMPORT 66/20/0
METALLURGICAL COAL 94.6
702/397/584
PETROCHEMICALS 84.4/17.7/17.1
REFINED OIL /GAS/COAL 617.6/379.3/432.3
24.5
40.3
7.2
1.2
3.0
4.76
47.6
6.2
4.9
1.9
87.3
5.65
20.5
14
12.7
1.28
1.4
1.32
0.48
2.5
2.2
2.2
0.73
6.05
429
TOTAL MATERIAL USE, 10⁹ Kg
RENEWABLE FRACTION

	PRINTING & PUBLISHING	CONTAINERS & PACKAGING	FABRICS	BUILDING & CONSTRUCTION	CHEMICALS	TRANSPORTATION	DURABLE GOODS
TOTAL MATERIAL USE, 10^9 Kg	24.5	54.5	5.3	952		22.3	24.1
RENEWABLE FRACTION	0.99	0.83	0.58	0.06		0.28	0.20

NOTES
1. SOLID ELEMENT DENOTES A REAL ACTIVITY.
2. MAJOR MATERIAL FLOWS ARE INDICATED IN 10^9 KILOGRAMS DELIVERED BY ACTIVITY.
3. SOME DATA ON THIS CHART ARE DERIVED FROM ENGINEERING ESTIMATES.
4. OTHER MATERIALS INCLUDING ALLOYING AND PRECIOUS ELEMENTS TO BE ADDED.

use and substitution of alternative resources. This was done by using the perturbation technique in which incremental effects of the substitution were analyzed for each scenario with respect to the material flows and attendant energy, economic, and environmental implications indicated on the RMS diagram and backup data sheets.

The technique of perturbation analysis involves the following steps after the definition of a base, or most likely case, in the RMS format:

1. Analysis of the demands for the specific basic chemical involved in a utilization or substitution case or scenario;
2. Definition of conventional petroleum processes to be used in the trajectory from the resource to the specific end use (definition of losses, energy, and capital requirements, and specific environmental issues and problems that arise);
3. Revision of flows through the affected trajectories in the RMS to reflect the substitution of alternative resources and feedstocks for basic chemicals and/or new processes;
4. Accumulation and tabulation of resource, energy, and environmental consequences of the modified utilization or substitution; and
5. Evaluation of specific environmental issues and problems that arise in the more intensive use of coal, shale oil, and renewable resources as feedstocks for basic chemicals.

The parameters and technical characteristics that describe conversion processes were defined externally to the RMS by MATHTECH experts and consultants with a process background. The objective of the RMS format was to capture that information and related environmental problems specific to portions of the feedstock cycle. In addition to serving an integrating role of this Mini-Assessment, the format may be employed to integrate new information as it becomes available in the future.

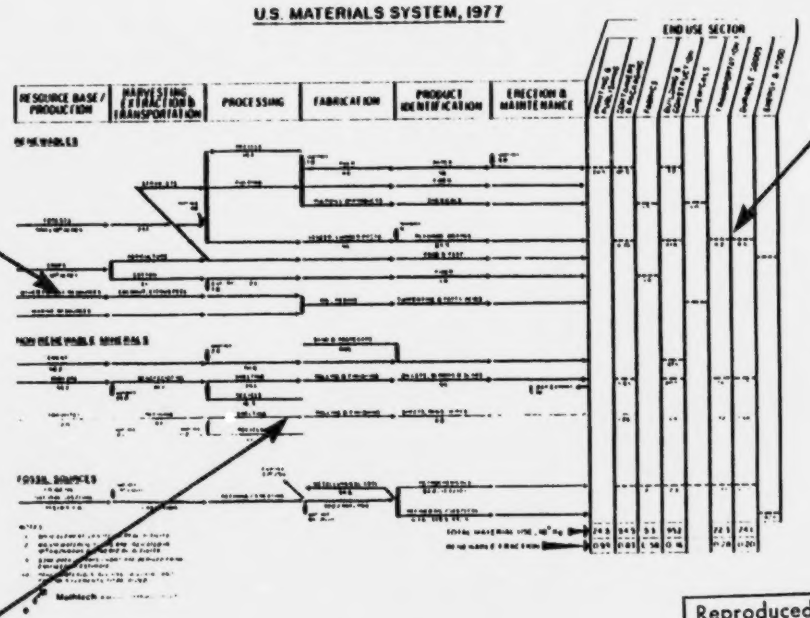
The further development of the Reference Materials System as a framework for assessments would involve the development of a more complete data base on chemicals and materials. Figure A.3 illustrates how data from a variety of sources may be mapped into various portions of the system. Information on the resource base including prices and quantities may be assembled from sources such as the Department of Interior's Computerized Resources Information Base (CRIB). Data on conversion processes may be extracted from Ayres Materials - Process - Product Model, SEAS, and other process models of specific industries. Finally, data on market demands and substitution patterns can be gleaned from the BEA and BLS input/output models and from technical and econometric models of specific sectors.

A computer software package, the Energy and Materials Network Simulator (ENMAT), may be employed for impact analyses using the Reference Materials System. Examples of the type of data elements that may be associated with specific links and sectors of the REFERENCE MATERIALS SYSTEM to support integrated policy analyses are as follows:

- RESOURCE BASE
  - Quantity of resources
  - Location
  - Quality
  - Cost of recovery

Figure A.3. Reference Materials System: Information Framework for Chemicals and Materials Assessment

(Integrated System Defined at Level of Plant, Region or Nation)


U.S. MATERIALS SYSTEM, 1977
RESOURCE BASE/ PRODUCTION
HARVESTING EXTRACTION & TRANSPORTATION
PROCESSING
FABRICATION
PRODUCT IDENTIFICATION
ERECTION & MAINTENANCE
END USE SECTOR
RENEWABLES
NONRENEWABLE MINERALS
FOSSIL SOURCES

RESOURCE BASE

- PRICES
- QUANTITIES
- CHARACTERISTICS

CHEMICAL AND MATERIAL MARKETS

- SECTORAL DEMANDS
- SUBSTITUTION ESTIMATES
- MARKET SHARES

PROCESSING AND CONVERSION INFRASTRUCTURE

- TECHNICAL CHARACTERISTICS
- CAPITAL COST, VARIABLE COST
- ENVIRONMENTAL COEFFICIENTS
- WASTES

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- PROCESSES, SUPPLY, AND END USE
  - Energy delivered, annual rate and peak
  - Efficiency
  - Ancillary fuel and resource inputs

- DEMAND
  - Demographics
  - Income groupings
  - Per capita use of energy services
  - Price and income elasticities
  - Industrial structure
  - Transportation patterns
  - Building stock
  - Appliance stock

- ECONOMICS
  - Capital cost of energy supply and use technology
  - Operating cost

- LABOR AND MATERIALS
  - Labor requirements for process
  - Major material requirement

- INSTITUTIONAL AND REGULATORY
  - Industrial concentration in various sectors
  - Regulations that affect various sectors
  - Research and development activities

- ENVIRONMENTAL
  - WATER: Acids
    - Bases
    - Phosphates
    - Nitrates
    - Dissolved solids
    - Suspended solids
    - Organics
    - BOD and COD
  - AIR: Particulates
    - Nitrogen oxides
    - Sulfur dioxide
    - Hydrocarbons
    - Carbon monoxide
    - Carbon dioxide
    - Aldehydes
  - OTHER: Solid waste
    - Land use
    - Occupational hazards
    - Radioactive wastes
    - Tritium
    - Krypton

APPENDIX B. UNDERLYING ASSUMPTIONS

B.1. Summary of Energy Scenario

In its Annual Report to Congress, the DOE-Energy Information Administration includes projections of energy production for the short-, mid-, and long-term. For purposes of comparison with chemical feedstock requirements, we utilize the long term, high oil price scenario of the 1979 Annual Report. In this scenario the real price of oil rises to $60 per barrel by the year 2000 (in 1979 dollars). The total domestic demand for energy (domestic production plus net imports) increases at an annual average rate of 1.5 percent from 1978 levels to 110.6 quadrillion BTUs (Quads) per year in 2000. Projections for energy production in the year 2000 as well as actual production in 1978 are presented in Table B.1.

The high price for crude oil encourages the development of several alternative energy sources, particularly synthetic fuels. One of the major assumptions which underlies this scenario is that synthetic liquids production will grow at a high rate in response to current policies and that these liquids will replace some imports as the marginal source of crude oil. Nevertheless, the EIA Projection for 2000 falls

Table B.1: U.S. Energy Consumption*

(Quadrillion BTU per year)

U.S. Production	1978		2000*	
Coal	15		37.9	
Natural Gas	19.5		16.2	
conventional		18.6		12.8
enhanced recovery		0.9		3.3
syngas (high BTU)		0		0.1
(imports)	(0.9)		(0.6)	
Oil (domestic)	20.7		24.2	
conventional		20.1		16.6
enhanced recovery		0.6		2.6
shale		0		2.7
syn crude (coal)		0		1.0
methanol (coal)		0		0.3
boiler fuel (coal)		0		0.2
alcohol (biomass)		0		0.8
(imports)	(17.1)		(8.4)	
Nuclear	3.0		11.3	
Other	4.3		12.0	
Total Domestic:	62.5		101.6	
Imports	18.0		9.0	
Total Supply:	80.5		110.6	

*Source: DOE-EIA 1979 Annual Report; primarily derived from Table 5.4, p.165, with exception of projected oil production which is from Table 5.19, p.205.

** High oil price scenario used; price reaches $60 per barrel by 2000 (in $1979).

short of the Carter Administration's goal of five Quads of shale oil and coal liquids by 1992. The demand for liquid fuels in end-use sectors increases significantly from about 30 Quads in 1980 to 45 Quads in 2000. A large part of this increase in demand is satisfied by shale oil and synthetic liquids produced form coal and biomass. In this scenario ten percent of total liquids production is composed of synthetic coal and biomass liquids by the year 2000. The synthetic fuels plants are expected to be "mine-mouth plants" utilizing western coal reserves. Hence, the potential sources of chemical feedstocks are expected to be located in the West.

The production of alcohol from biomass is also significant in this scenario. Alcohol from biomass represents 38 percent of total synthetic liquids in 2000 (0.8 Quads per year). This scenario is sensitive to the price of oil: production of alcohol from biomass for the high oil price is almost three times that for the low oil price scenario.

Coal production is expected to more than double by 2000 over 1978 levels. This increase is expected to occur independently of the rise in oil prices because of cost advantages even at the lower oil cost. In addition, coal use by electric utilities is expected to increase due to restrictions on oil and gas use in new generating units by the Powerplant and Industrial Fuel Use Act. Because of regional environmental standards (e.g., in the Northeast) and transportation costs, electricity generation is expected to gravitate toward the western coal sources. Thus, in addition to the synfuels programs, this trend may lead to increased demands on the environmental capacities of the western coal-producing states.

The high oil price scenario of the EIA 1979 Annual Report is believed to be reasonable for our purposes. Recent increases indicate that oil prices will indeed rise at a rate well above inflation (the $60 price in 2000 represents an annual average growth rate of five percent above inflation over a 1979 price of $21.50). Because of recent price increases, the EIA is revising the forecasts for the next iteration to include the present "high" forecast as a midprice scenario.

There are additional factors which may influence this projection, and its effects on the chemical industry, in addition to the government policies discussed below.

First, unconventional sources of natural gas (gas dissolved in geopressured brine or not associated with oil reservoirs) could be commercialized in this country.

Second, major new hydrocarbon sources may be developed in nearby countries. Venezuelan reserves of heavy crude oil are three times the reserves in Saudi Arabia. Canadian heavy oil and tar sands are, in turn, twice Venezuela's. The Canadian tar sand reserve, representing 900 billion barrels of oil, is already being exploited, but weather and handling the tailings are major impediments. The U.S. tar sands reserve of 25 to 36 billion barrels, half in Utah, is much less accessible and is unlikely to be recovered soon, if at all (1).

B.2. Federal Policy and Regulation

The greatest influences on the choice of chemical feedstocks will be actions of the U.S. government: laws, regulations, taxes, incentives, and subsidies. A full accounting would be a major study in itself, but the following (in no particular order) could have major impacts:

- Government support of research and commercialization of ethanol, shale and coal conversion technologies;
- Government support of research into conversion of the products and by-products of those technologies into chemicals;
- Government support of long-term basic academic research in chemistry, materials, etc. (2);
- Accelerated deregulation of oil and natural gas prices;
- Tax policy on energy exploration and exploitation;
- Subsidies for ethanol and other alternative fuels (e.g., on interest rates, selling price);
- Regulation of the use of particular energy sources by utilities and various industries;
- Government support of heating fuel conservation (e.g., building codes, maximum temperatures);
- Government influences on gasoline consumption (e.g., gasoline tax, miles per gallon requirements, actions to preserve the American car manufacturers);
- Government policy on the priority of feedstocks over fuel use of limited oil and gas (currently no priority) and eventually of oil over alternative fuel/feedstock sources;
- Encouragement of brokers and jobbers to engage in recycling of chemicals, such as solvents and off-grade resins, perhaps with "toxic waste prevention" credits;
- U.S. trade agreements, or embargoes, tariff regulations, exchange rates (change and stability), and transnational corporation internal transfers; and U.S. policy on domestic energy prices, as they affect the international trade in chemicals;

- Tax, licensing and patent laws (2) and international agreement and cooperation or lack thereof, as they affect the international disposition of chemical manufacturing;
- Stability of government policy and action on all energy questions;
- National and private forest management policies;
- Environmental regulation concerning "acid rain," strip mining, western water usage, permit procedures; and
- others.

It would be impossible to predict the net outcome; many policies will be enacted without chemicals being considered at all. Further, new decisions will continually be made, and changed, by the administration and by Congress. Thus the lead time which this Mini-Assessment assumes will best be used to organize monitoring rather than predictive procedures.

REFERENCES

(1) Marcus, J. Sandy Oil at the Margin. Technology Review, February/March 1981. p. 85.

(2) Shapiro, I.S. Future Sources of Organic Raw Materials. Science, Oct. 20, 1978. pp. 287-289.

APPENDIX C. RMS SCENARIO DETAILS

C.1. System R-1980

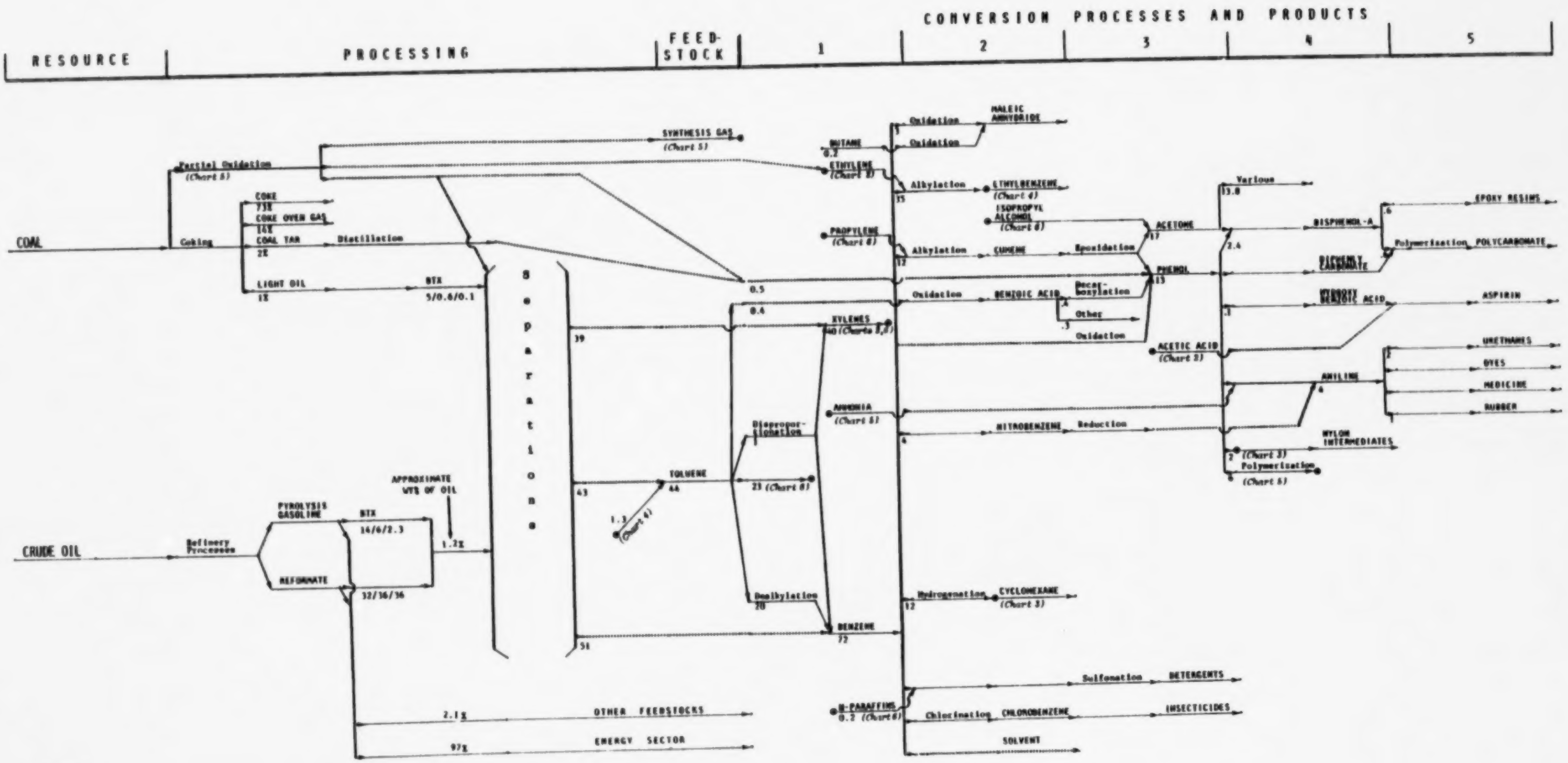
After a detailed description of System R-1980 Chart 1: Benzene there will follow a guide to noteworthy features of Charts 2 through 6. Despite their complexity, these charts do not describe the organic chemical industry exhaustively. Benzene alone has hundreds of derivatives. However, the charts display the major uses of and connections between the basic chemicals.

On an RMS Chart, dots (nodes) represent a process or a product, with the label appearing on the following line segment -- in capitals for a chemical, in lower case for a process. Dotted lines transport chemicals through chart space where no chemical processing is required. For instance, secondary chemical nitrobenzene is reduced to aniline, a quarternary chemical because it has an alternative production route with an additional step. Dashed lines represent processes which have been commercial but are no longer used. Large dots, with a nearby chart reference in parentheses, indicate connections between charts.

Benzene comes from two resources, coal and crude oil, shown on the left of Chart R-1980.1. The by-products of

SYSTEM R-1980

CHART 1: BENZENE


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL
Partial Oxidation
(Chart 5)
Coking
COKE
73%
COKE OVEN GAS
14%
COAL TAR
2%
Distillation
LIGHT OIL
1%
BTX
5/0.6/0.1
SYNTHESIS GAS
(Chart 5)
CRUDE OIL
Refinery Processes
PYROLYSIS GASOLINE
REFORMATE
BTX
14/6/2.3
32/16/16
APPROXIMATE WT% OF OIL
1.2%
2.1%
OTHER FEEDSTOCKS
97%
ENERGY SECTOR
Separations
39
43
51
1.3
(Chart 4)
TOLUENE
44
0.5
0.4
Disproportionation
23 (Chart 8)
Dealkylation
20
XYLENES
40 (Charts 5,8)
BENZENE
72
BUTANE
0.2
ETHYLENE
(Chart 8)
PROPYLENE
(Chart 8)
AMMONIA
(Chart 5)
N-PARAFFINS
0.2 (Chart 6)
3
15
12
4
12
Oxidation
Oxidation
MALEIC ANHYDRIDE
Alkylation
ETHYLBENZENE
(Chart 4)
ISOPROPYL ALCOHOL
(Chart 8)
Alkylation
CUMENE
Epoxidation
Oxidation
BENZOIC ACID
Decarboxylation
.4
Other
.3
Oxidation
NITROBENZENE
Reduction
Hydrogenation
CYCLOHEXANE
(Chart 3)
Sulfonation
DETERGENTS
Chlorination
CHLOROBENZENE
INSECTICIDES
SOLVENT
ACETONE
17
PHENOL
13
ACETIC ACID
(Chart 2)
Various
13.0
2.4
.1
2
(Chart 3)
Polymerization
(Chart 6)
BISPHENOL-A
DIPHENYL CARBONATE
HYDROXY BENZOIC ACID
ANILINE
4
NYLON INTERMEDIATES
.6
Polymerization
POLYCARBONATE
EPOXY RESINS
ASPIRIN
2
URETHANES
DYES
MEDICINE
RUBBER
1

NOTES:

1. Numbers are millions of kilogram moles per year and are estimates of average flows for 1979 through 1981.
2. Each node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

ALTERNATIVE SOURCES

CHART 5: GASOLINE
CHART 7: BTX, PHENOL
CHART 8: BTX, PHENOLS, GASOLINE & FUELS
CHART 9: BTX, PHENOL, ACETONE, GASOLINE

coal coking now provide only a small fraction of chemical feedstocks, whereas once they dominated a much smaller industry. The light oil fraction is predominately benzene, with some toluene and xylene. The refining of crude oil provides two principal sources of aromatics. The aromatics separated from pyrolysis gasoline are two-thirds benzene, those from reformate, are approximately equimolar in each principal aromatic. The aromatics in these two streams comprise about 1.2 percent of all crude oil refined in the United States. Other feedstocks from crude oil use an additional 2.1 percent. After the three chemicals are separated, about half of the toluene (a feedstock) is dealkylated to benzene and a small amount is catalytically reacted (disproportionated) to xylene and benzene. The latter are thus primary chemicals.

To display adequately the steps between feedstocks and finished chemicals, five conversion process stages are shown. Even so, some multi-step syntheses have been lumped together and not all of the sequential intermediates are shown.

Further, some chemical substances occur at different steps in the various conversion sequences. For instance, in Chart 1, phenol can be formed by the direct oxidation of feedstock toluene, or of primary-chemical benzene, or as the tertiary product of the epoxidation of cumene. However, the last of those reactions predominates, and phenol is presented as a tertiary chemical throughout the charts.

Typically the trajectories end in connections to other charts, in net exports, or in a finished chemical product. For the most part, the trajectories do not culminate in final marketed products, although some will be obvious.

Also shown on Chart R-1980.1 (as well as 2 through 6) is a list of those chemicals which in the future may be derived from the alternative sources shown on Charts R-1980.5 and 7 through 10.

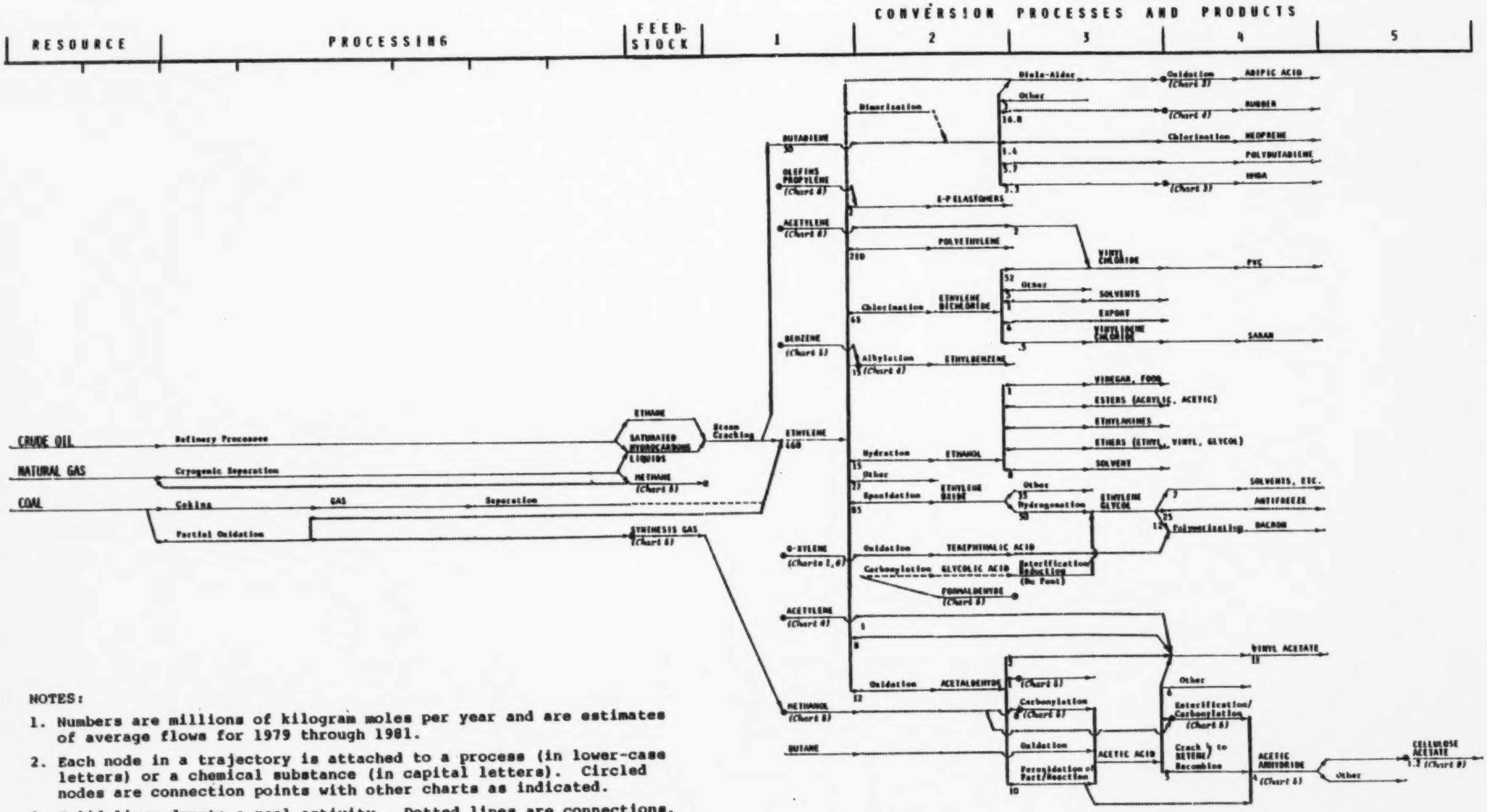
As shown on Chart R-1980.2, ethylene is about sixty percent derived from natural gas liquids, and nearly eighty percent is consumed in its three largest uses - polyethylene, ethylene oxide and ethylene dichloride. This chart also shows butadiene which is an important coproduct with ethylene and propylene (R-1980.6) from the steam cracking of saturated hydrocarbons.

Chart R-1980.3:Cyclohexane primarily shows the complex multitude of chemical paths to two varieties of nylon. Cyclohexane must compete not only with another benzene derivative, phenol, but with two of the coproducts from steam cracking, butadiene and propylene (as acrylonitrile).

Ethylbenzene is almost totally converted to styrene, as shown on Chart R-1980.4, but there are two principal pathways. The older process is simple dehydrogenation. A more recent process involves the simultaneous conversion of propylene into propylene oxide and ethylbenzene into an alcohol by an epoxidation reaction and then dehydration of the alcohol. Styrene uses are grouped as plastic resins and synthetic rubbers.

SYSTEM R-1980

CHART 2: ETHYLENE


CONVERSION PROCESSES AND PRODUCTS
RESOURCE
PROCESSING
FEED-STOCK
1
2
3
4
5
CRUDE OIL
NATURAL GAS
COAL
Refinery Processes
Cryogenic Separation
Coking
GAS
Separation
Partial Oxidation
ETHANE
SATURATED HYDROCARBONS
LIQUIDS
METHANE (Chart 8)
SYNTHESIS GAS (Chart 8)
Steam Cracking
BUTADIENE 30
OLEFINS PROPYLENE (Chart 8)
ACETYLENE (Chart 8)
BENZENE (Chart 1)
ETHYLENE 460
O-XYLENE (Charts 1,8)
ACETYLENE (Chart 4)
METHANOL (Chart 8)
BUTANE
Dimerization
Diels-Alder
Other
16.8
1.4
3.7
3.3
Oxidation (Chart 3)
ADIPIC ACID
(Chart 4)
RUBBER
Chlorination
NEOPRENE
POLYBUTADIENE
(Chart 3)
HMDA
2
E-P ELASTOMERS
2
POLYETHYLENE
210
VINYL CHLORIDE
PVC
52
Other
5
SOLVENTS
1
EXPORT
6
VINYLIDENE CHLORIDE
.5
SARAN
Chlorination
ETHYLENE DICHLORIDE
65
Alkylation
15 (Chart 4)
ETHYLBENZENE
1
VINEGAR, FOOD
ESTERS (ACRYLIC, ACETIC)
ETHYLAMINES
ETHERS (ETHYL, VINYL, GLYCOL)
SOLVENT
8
Hydration
ETHANOL
15
Other
27
Epoxidation
ETHYLENE OXIDE
85
Other
35
Hydrogenation
50
ETHYLENE GLYCOL
3
SOLVENTS, ETC.
25
ANTIFREEZE
12
Polymerizing
DACRON
Oxidation
TEREPHTHALIC ACID
Carbonylation
GLYCOLIC ACID
Esterification/Reduction (Du Pont)
FORMALDEHYDE (Chart 8)
1
8
VINYL ACETATE
11
Oxidation
ACETALDEHYDE
12
3
1 (Chart 5)
Carbonylation
8 (Chart 5)
Oxidation
Peroxidation of Part/Reaction
10
ACETIC ACID
Other
6
Esterification/Carbonylation (Chart 5)
Crack ½ to KETENE/Recombine
5
ACETIC ANHYDRIDE
4 (Chart 5)
CELLULOSE ACETATE
.3 (Chart 9)
Other

NOTES:

1. Numbers are millions of kilogram moles per year and are estimates of average flows for 1979 through 1981.
2. Each node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

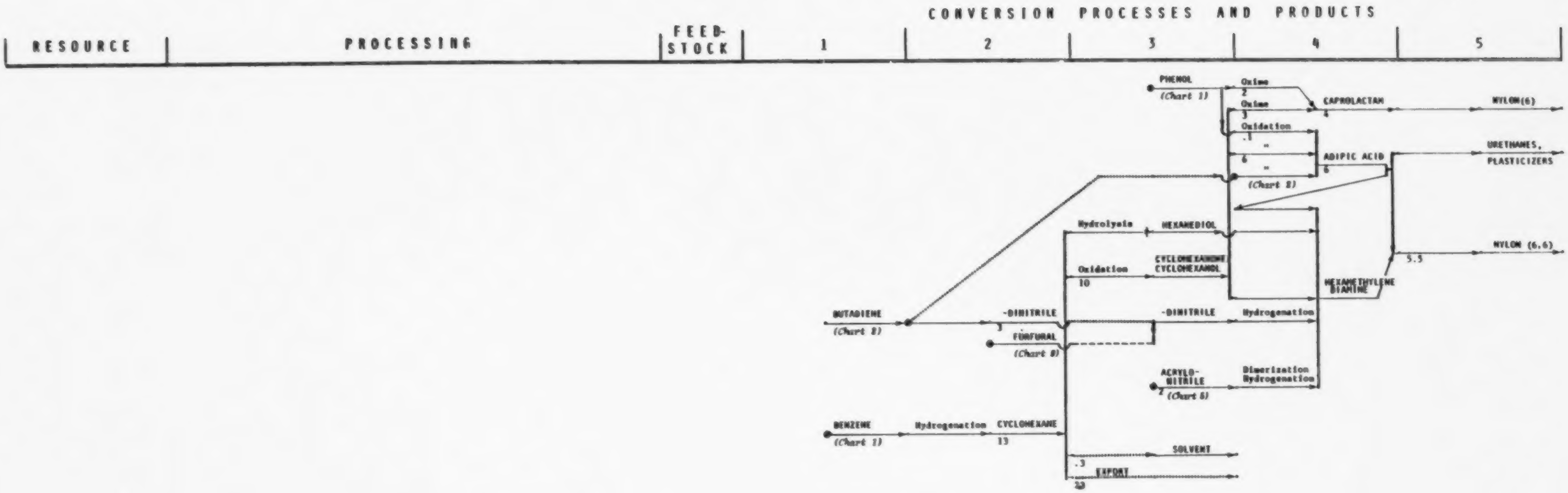
ALTERNATIVE SOURCES

CHART 5: ETHYLENE et al., ACETIC ACID/ANHYDRIDE

CHART 7: ETHANE

CHART 9: ETHANOL

SYSTEM R-1980
CHART 3: CYCLOHEXANE


CONVERSION PROCESSES AND PRODUCTS
RESOURCE
PROCESSING
FEED-STOCK
1
2
3
4
5
PHENOL
(Chart 1)
Oxime
2
Oxime
3
Oxidation
.1
"
6
"
(Chart 2)
CAPROLACTAM
4
NYLON(6)
ADIPIC ACID
6
URETHANES,
PLASTICIZERS
NYLON (6,6)
5.5
Hydrolysis
HEXANEDIOL
Oxidation
10
CYCLOHEXANONE
CYCLOHEXANOL
HEXAMETHYLENE DIAMINE
BUTADIENE
(Chart 2)
-DINITRILE
3
FURFURAL
(Chart 8)
-DINITRILE
Hydrogenation
ACRYLO-NITRILE
2
(Chart 5)
Dimerization
Hydrogenation
BENZENE
(Chart 1)
Hydrogenation
CYCLOHEXANE
13
SOLVENT
.3
EXPORT
23

NOTES:

1. Numbers are millions of kilogram moles per year and are estimates of average flows for 1979 through 1981.
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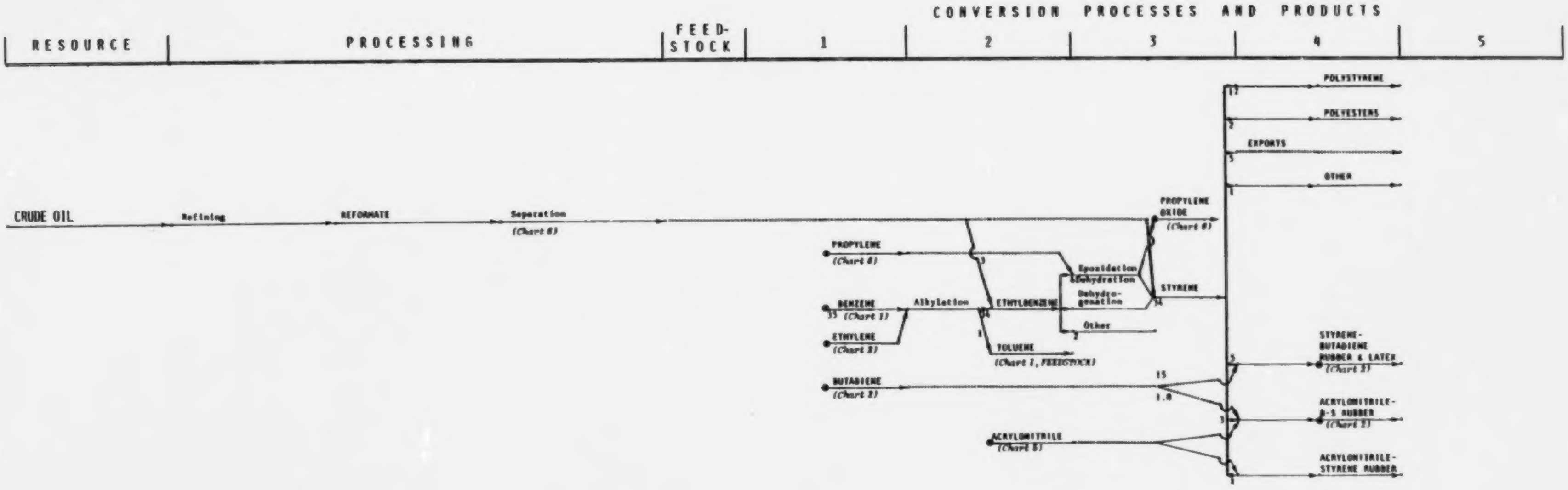
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

ALTERNATIVE SOURCES

CHART 9: FURFURAL, PHENOL

SYSTEM R-1980

CHART 4: ETHYLBENZENE, STYRENE


CONVERSION PROCESSES AND PRODUCTS
RESOURCE
PROCESSING
FEED-STOCK
1
2
3
4
5
CRUDE OIL
Refining
REFORMATE
Separation
(Chart 6)
PROPYLENE
(Chart 6)
BENZENE
35 (Chart 1)
ETHYLENE
(Chart 2)
BUTADIENE
(Chart 3)
Alkylation
3
14
1
ETHYLBENZENE
TOLUENE
(Chart 1, FEEDSTOCK)
ACRYLONITRILE
(Chart 5)
Epoxidation
Dehydration
Dehydro-genation
Other
2
PROPYLENE OXIDE
(Chart 6)
STYRENE
14
15
1.0
17
POLYSTYRENE
2
POLYESTERS
5
EXPORTS
1
OTHER
5
STYRENE-BUTADIENE RUBBER & LATEX
(Chart 2)
3
ACRYLONITRILE-B-S RUBBER
(Chart 2)
1
ACRYLONITRILE-STYRENE RUBBER

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At present, almost all synthesis gas comes from natural gas (Chart R-1980.5). Ammonia, the predominate use, and its further derivatives urea and nitric acid are non-organic chemicals but are nevertheless closely related to the organic chemical industry in practice. The lower part of the chart features methanol and other organic chemicals which are formed by recombining the CO and H_2 with other oxygenated chemicals to build up longer carbon chains.

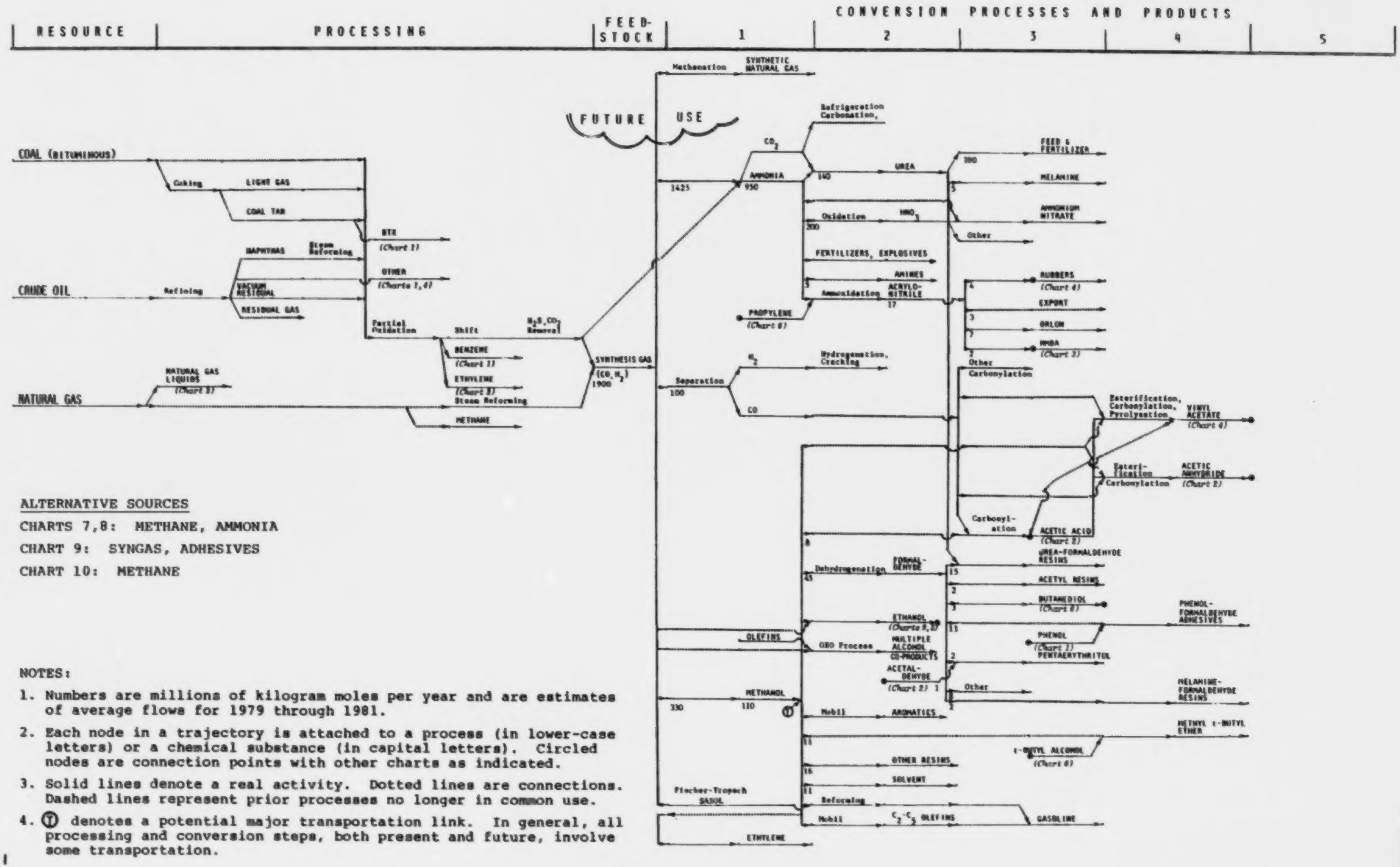
Chart R-1980.6 shows a wide variety of chemical products and the prevalence of connections: chemicals from multiple sources (e.g., acetylene, naphthalene, and aromatics from both oil and coal), joined in products (e.g., polybutylene terephthalate), and competing for products (e.g., o-xylene or naphthalene to phthalic anhydride, formaldehyde or acetylene to 1,4-butanediol, or the three processes for propylene oxide).

Charts R-1980.7, 8, and 10 are presented here only to provide a complete set of charts for reference. They, and most of the detail on Chart 9, are described and discussed under the appropriate scenarios. Chart R-1980.9 at the top shows the route to the acetate fibers and also shows the by-products recovered from the pulp and paper industry -- artificial vanilla and the controversial drug DMSO.

The major basic chemicals demonstrate the interrelated sources and uses of organic chemicals. For instance, the fourth largest use of ethylene is to alkylate one-half of the total benzene consumed. The product, ethylbenzene , is dehydrogenated to styrene which finds its largest use in

SYSTEM R-1980

CHART 5: SYNTHESIS GAS


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL (BITUMINOUS)
Coking
LIGHT GAS
COAL TAR
BTX
(Chart 1)
NAPHTHAS
Steam Reforming
OTHER
(Charts 1,4)
CRUDE OIL
Refining
VACUUM RESIDUAL
RESIDUAL GAS
Partial Oxidation
Shift
H_2S, CO_2 Removal
BENZENE
(Chart 1)
ETHYLENE
(Chart 3)
Steam Reforming
METHANE
NATURAL GAS LIQUIDS
(Chart 3)
NATURAL GAS
SYNTHESIS GAS
(CO, H_2)
1900
FUTURE USE
Methanation
SYNTHETIC NATURAL GAS
CO_2
Refrigeration Carbonation,
AMMONIA
1425
950
140
UREA
300
FEED & FERTILIZER
MELAMINE
5
Oxidation
HNO_3
200
AMMONIUM NITRATE
Other
FERTILIZERS, EXPLOSIVES
AMINES
5
Ammoxidation
ACRYLO-NITRILE
17
PROPYLENE
(Chart 6)
4
RUBBERS
(Chart 4)
EXPORT
3
ORLON
7
MMBA
(Chart 3)
2
Separation
100
H_2
Hydrogenation, Cracking
CO
Other Carbonylation
Esterification, Carbonylation, Pyrolyzation
VINYL ACETATE
(Chart 4)
Esteri-fication
Carbonylation
ACETIC ANHYDRIDE
(Chart 2)
Carbonyl-ation
ACETIC ACID
(Chart 2)
8
UREA-FORMALDEHYDE RESINS
Dehydrogenation
FORMAL-DEHYDE
45
15
ACETYL RESINS
2
BUTANEDIOL
(Chart 6)
3
PHENOL-FORMALDEHYDE ADHESIVES
ETHANOL
(Charts 9,2)
13
PHENOL
(Chart 1)
OLEFINS
OXO Process
MULTIPLE ALCOHOL CO-PRODUCTS
2
PENTAERYTHRITOL
ACETAL-DEHYDE
(Chart 2)
1
Other
MELAMINE-FORMALDEHYDE RESINS
2
METHANOL
330
110
Ⓣ
Mobil
AROMATICS
METHYL t-BUTYL ETHER
11
t-BUTYL ALCOHOL
(Chart 6)
OTHER RESINS
16
SOLVENT
11
Fischer-Tropsch SASOL
Reforming
GASOLINE
Mobil
C_2-C_5 OLEFINS
ETHYLENE

ALTERNATIVE SOURCES

CHARTS 7,8: METHANE, AMMONIA

CHART 9: SYNGAS, ADHESIVES

CHART 10: METHANE

NOTES:

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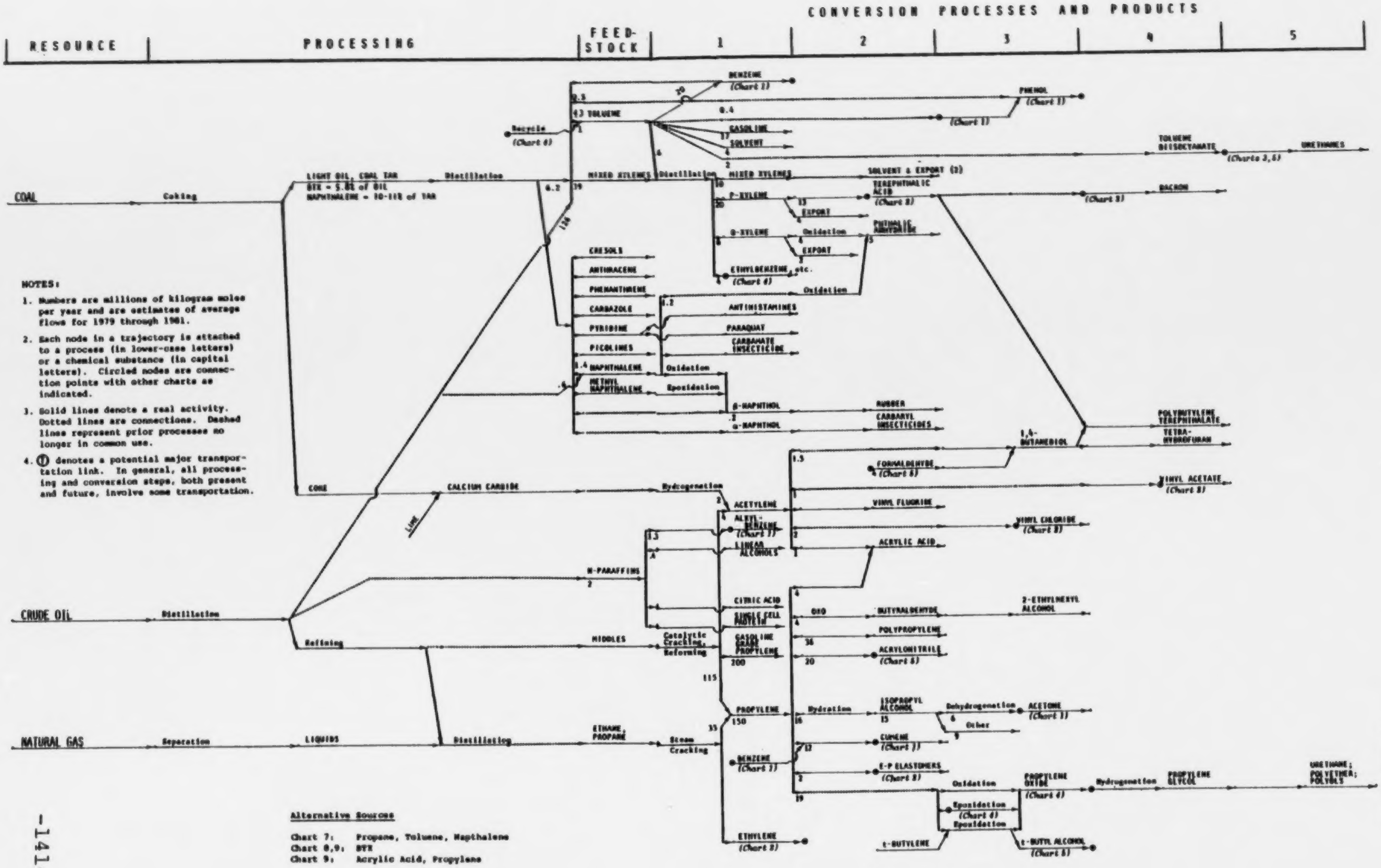
SYSTEM R-1980

CHART 6: OTHER BASIC CHEMICALS


CONVERSION PROCESSES AND PRODUCTS
RESOURCE
PROCESSING
FEED-STOCK
1
2
3
4
5
COAL
Coking
LIGHT OIL, COAL TAR
BTX = 5.8% of OIL
NAPHTHALENE = 10-11% of TAR
Distillation
COKE
CALCIUM CARBIDE
LIME
Recycle
(Chart 4)
TOLUENE
MIXED XYLENES
Distillation
BENZENE
(Chart 1)
PHENOL
(Chart 1)
GASOLINE
SOLVENT
TOLUENE DIISOCYANATE
(Charts 3,5)
URETHANES
SOLVENT & EXPORT (2)
P-XYLENE
TEREPHTHALIC ACID
(Chart 8)
DACRON
EXPORT
O-XYLENE
Oxidation
PHTHALIC ANHYDRIDE
ETHYLBENZENE, etc.
CRESOLS
ANTHRACENE
PHENANTHRENE
CARBAZOLE
PYRIDINE
PICOLINES
NAPHTHALENE
METHYL NAPHTHALENE
Epoxidation
ANTIHISTAMINES
PARAQUAT
CARBAMATE INSECTICIDE
β-NAPHTHOL
α-NAPHTHOL
RUBBER
CARBARYL INSECTICIDES
POLYBUTYLENE TEREPHTHALATE
TETRA-HYDROFURAN
1,4-BUTANEDIOL
FORMALDEHYDE
(Chart 5)
VINYL ACETATE
VINYL FLUORIDE
VINYL CHLORIDE
ACRYLIC ACID
Hydrogenation
ACETYLENE
ALKYL-BENZENE
(Chart 7)
LINEAR ALCOHOLS
N-PARAFFINS
CRUDE OIL
Distillation
Refining
MIDDLES
Catalytic Cracking, Reforming
CITRIC ACID
SINGLE CELL PROTEIN
GASOLINE GRADE PROPYLENE
OXO
BUTYRALDEHYDE
2-ETHYLHEXYL ALCOHOL
POLYPROPYLENE
ACRYLONITRILE
PROPYLENE
Hydration
ISOPROPYL ALCOHOL
Dehydrogenation
Other
ACETONE
CUMENE
E-P ELASTOMERS
PROPYLENE OXIDE
PROPYLENE GLYCOL
URETHANE; POLYETHER; POLYOLS
t-BUTYLENE
t-BUTYL ALCOHOL
NATURAL GAS
Separation
LIQUIDS
Distilling
ETHANE, PROPANE
Steam Cracking
ETHYLENE
(Chart 2)
6.2
39
126
43
2.5
0.4
20
17
4
2
10
30
13
1.2
1.4
.5
.2
1.3
2
200
115
150
35
36
20
16
15
6
9
12
19

NOTES:

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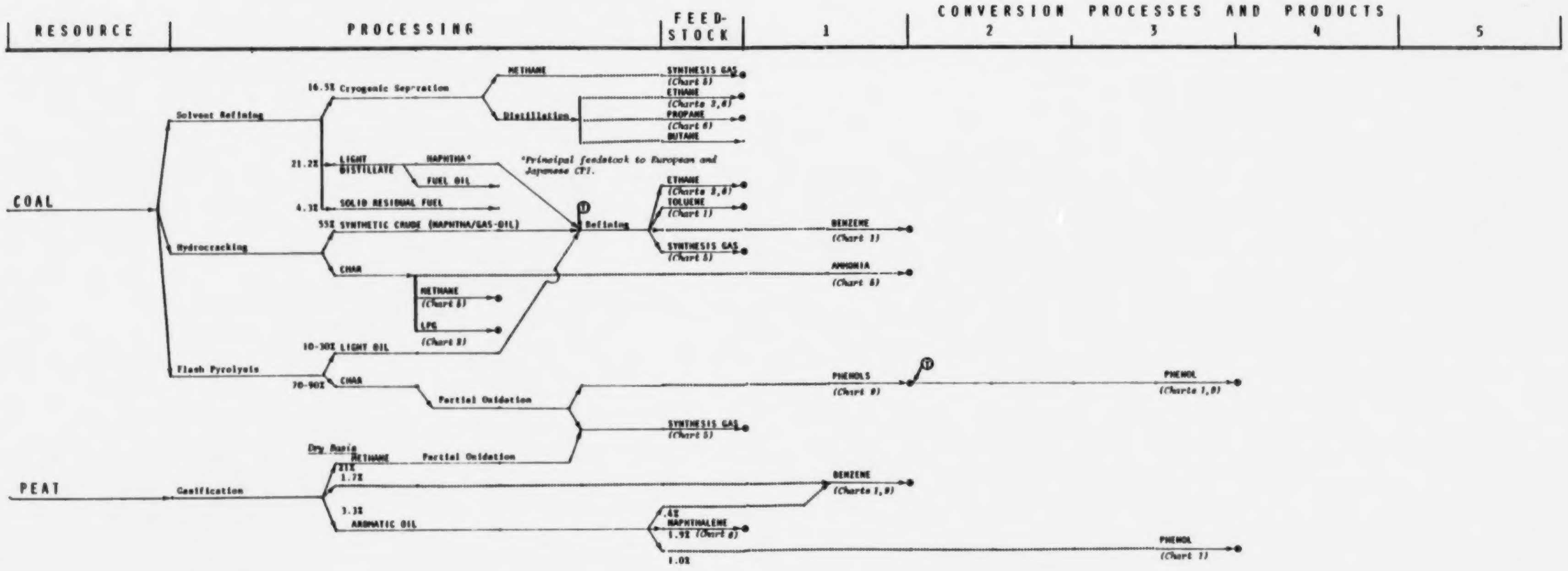
Alternative Sources

Chart 7: Propane, Toluene, Napthalene
Chart 8,9: BTX
Chart 9: Acrylic Acid, Propylene

SYSTEM R-1980
CHART 7: COAL, PEAT


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL
Solvent Refining
16.5% Cryogenic Sep'ration
METHANE
Distillation
SYNTHESIS GAS (Chart 5)
ETHANE (Charts 2,6)
PROPANE (Chart 6)
BUTANE
21.2% LIGHT DISTILLATE
NAPHTHA*
FUEL OIL
4.3% SOLID RESIDUAL FUEL
55% SYNTHETIC CRUDE (NAPHTHA/GAS-OIL)
Refining
ETHANE (Charts 2,6)
TOLUENE (Chart 1)
BENZENE (Chart 1)
SYNTHESIS GAS (Chart 5)
Hydrocracking
CHAR
AMMONIA (Chart 5)
METHANE (Chart 5)
LPG (Chart 2)
10-30% LIGHT OIL
Flash Pyrolysis
70-90% CHAR
Partial Oxidation
PHENOLS (Chart 8)
PHENOL (Charts 1,8)
SYNTHESIS GAS (Chart 5)
Dry Basis
METHANE
Partial Oxidation
21%
1.7%
PEAT
Gasification
BENZENE (Charts 1,8)
3.3%
AROMATIC OIL
.4%
NAPHTHALENE
1.9% (Chart 8)
1.0%
PHENOL (Chart 1)

*Principal feedstock to European and Japanese CTI.

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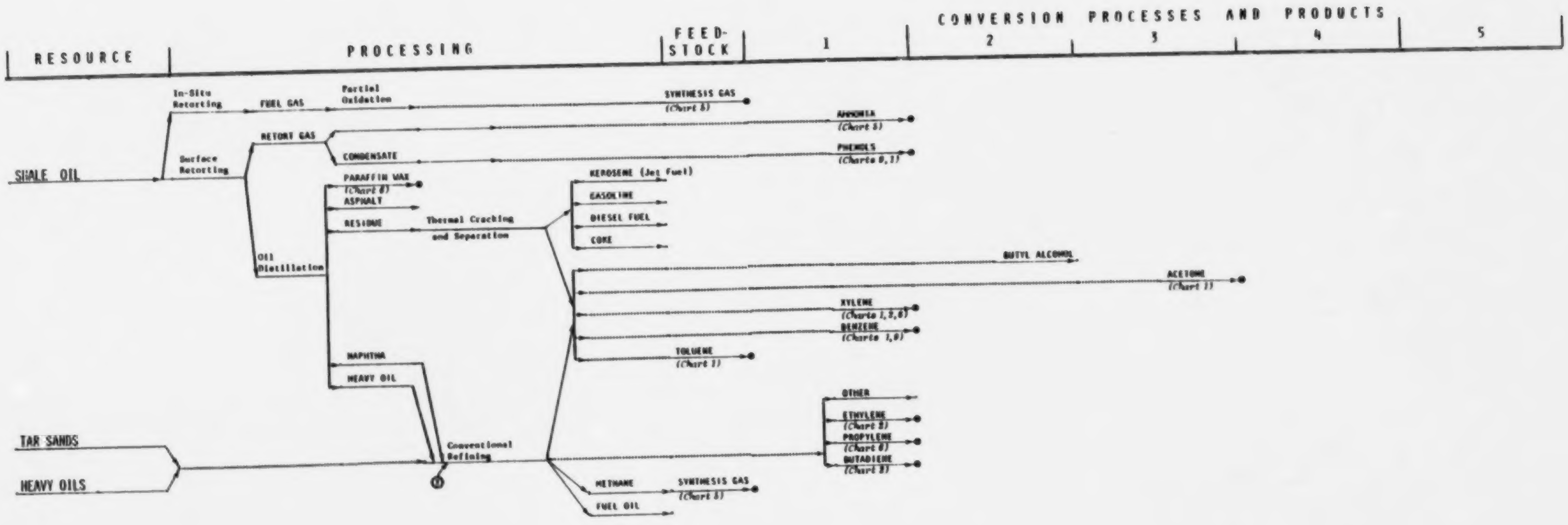
SYSTEM R-1980

CHART 8: SHALE OIL, TAR SAND, HEAVY OIL


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
SHALE OIL
In-Situ Retorting
FUEL GAS
Partial Oxidation
SYNTHESIS GAS (Chart 5)
Surface Retorting
RETORT GAS
AMMONIA (Chart 5)
CONDENSATE
PHENOLS (Charts 6,1)
Oil Distillation
PARAFFIN WAX (Chart 6)
ASPHALT
RESIDUE
Thermal Cracking and Separation
KEROSENE (Jet Fuel)
GASOLINE
DIESEL FUEL
COKE
BUTYL ALCOHOL
ACETONE (Chart 1)
XYLENE (Charts 1,2,6)
BENZENE (Charts 1,6)
TOLUENE (Chart 1)
NAPHTHA
HEAVY OIL
TAR SANDS
HEAVY OILS
Conventional Refining
Ⓣ
OTHER
ETHYLENE (Chart 2)
PROPYLENE (Chart 6)
BUTADIENE (Chart 3)
METHANE
SYNTHESIS GAS (Chart 5)
FUEL OIL

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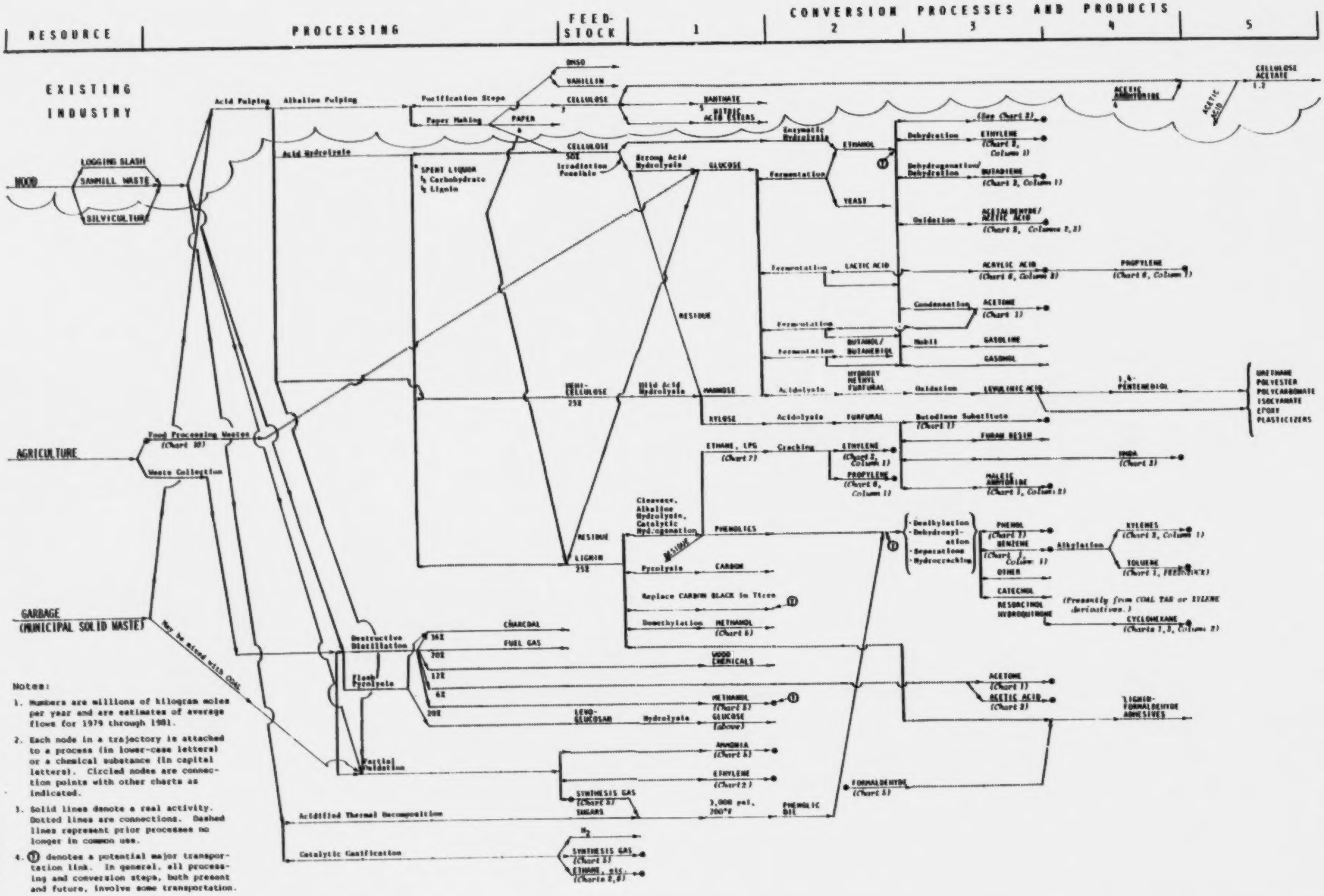
SYSTEM R-1980

CHART 9: WOOD, DRY BIOMASS


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
EXISTING INDUSTRY
WOOD
LOGGING SLASH
SAWMILL WASTE
SILVICULTURE
AGRICULTURE
GARBAGE (MUNICIPAL SOLID WASTE)
May be mixed with COAL
Acid Pulping
Alkaline Pulping
Acid Hydrolysis
Food Processing Wastes (Chart 10)
Waste Collection
Purification Steps
Paper Making
SPENT LIQUOR ½ Carbohydrate ½ Lignin
DMSO
VANILLIN
CELLULOSE
7
PAPER
6
CELLULOSE
50%
Irradiation Possible
XANTHATE
5
NITRIC ACID ESTERS
ACETIC ANHYDRIDE
4
ACETIC ACID
CELLULOSE ACETATE
1.2
Enzymatic Hydrolysis
Strong Acid Hydrolysis
GLUCOSE
Fermentation
ETHANOL
YEAST
T
(See Chart 2)
Dehydration
ETHYLENE (Chart 2, Column 1)
Dehydrogenation/ Dehydration
BUTADIENE (Chart 2, Column 1)
Oxidation
ACETALDEHYDE/ ACETIC ACID (Chart 2, Columns 2,3)
Fermentation
LACTIC ACID
ACRYLIC ACID (Chart 6, Column 3)
PROPYLENE (Chart 6, Column 1)
Condensation
ACETONE (Chart 1)
Fermentation
Fermentation
BUTANOL/ BUTANEDIOL
Mobil
GASOLINE
GASOHOL
RESIDUE
HEMI-CELLULOSE
25%
Mild Acid Hydrolysis
MANNOSE
XYLOSE
Acidolysis
HYDROXY METHYL FURFURAL
Oxidation
LEVULINIC ACID
1,4-PENTENEDIOL
URETHANE
POLYESTER
POLYCARBONATE
ISOCYANATE
EPOXY
PLASTICIZERS
Acidolysis
FURFURAL
Butadiene Substitute (Chart 1)
FURAN RESIN
HMDA (Chart 3)
MALEIC ANHYDRIDE (Chart 1, Column 2)
ETHANE, LPG (Chart 7)
Cracking
ETHYLENE (Chart 2, Column 1)
PROPYLENE (Chart 6, Column 1)
RESIDUE
LIGNIN
25%
Cleavage, Alkaline Hydrolysis, Catalytic Hydrogenation
RESIDUE
PHENOLICS
Pyrolysis
CARBON
Replace CARBON BLACK in Tires
T
Demethylation
METHANOL (Chart 5)
T
·Dealkylation
·Dehydroxylation
·Separations
·Hydrocracking
PHENOL (Chart 1)
BENZENE (Chart 1, Column 1)
OTHER
CATECHOL
RESORCINOL
HYDROQUINONE
Alkylation
XYLENES (Chart 2, Column 1)
TOLUENE (Chart 1, FEEDSTOCK)
(Presently from COAL TAR or XYLENE derivatives.)
CYCLOHEXANE (Charts 1,3, Column 2)
Destructive Distillation
Flash Pyrolysis
Partial Oxidation
36%
CHARCOAL
20%
FUEL GAS
12%
WOOD CHEMICALS
6%
20%
ACETONE (Chart 1)
ACETIC ACID (Chart 2)
METHANOL (Chart 5)
T
LEVO-GLUCOSAN
Hydrolysis
GLUCOSE (above)
LIGNIN-FORMALDEHYDE ADHESIVES
AMMONIA (Chart 5)
ETHYLENE (Chart 2)
SYNTHESIS GAS (Chart 5)
SUGARS
Acidified Thermal Decomposition
3,000 psi, 700°F
PHENOLIC OIL
FORMALDEHYDE (Chart 5)
Catalytic Gasification
H₂
SYNTHESIS GAS (Chart 5)
ETHANE, etc. (Charts 2,6)

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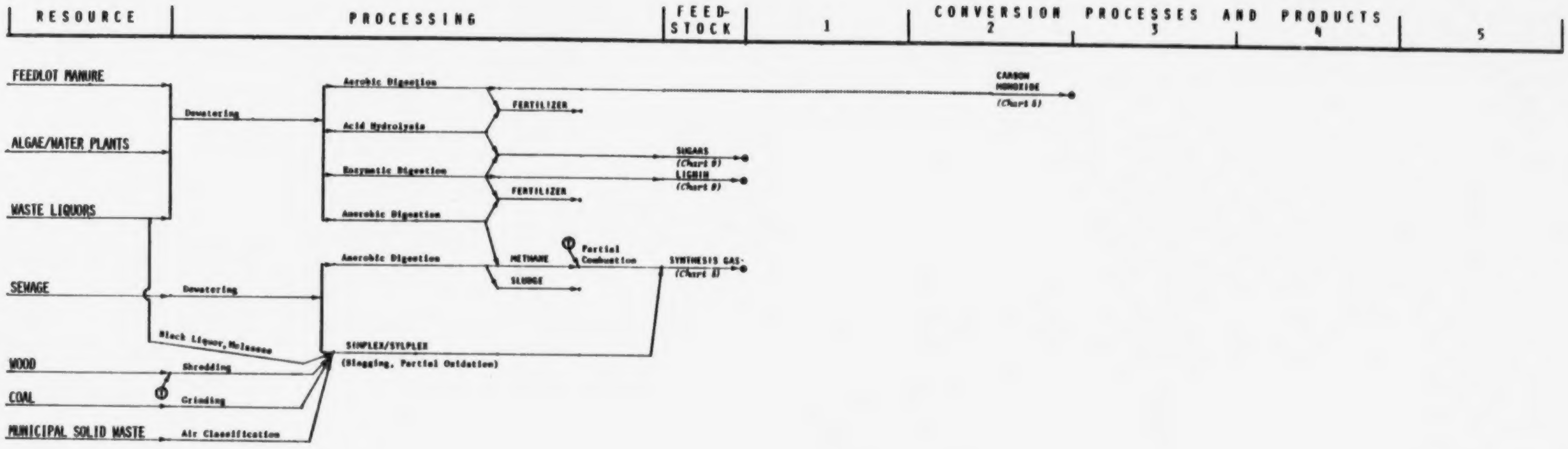
SYSTEM R-1980

CHART 10: WET BIOMASS


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
FEEDLOT MANURE
ALGAE/WATER PLANTS
WASTE LIQUORS
SEWAGE
WOOD
COAL
MUNICIPAL SOLID WASTE
Dewatering
Dewatering
Black Liquor, Molasses
Shredding
Grinding
Air Classification
Aerobic Digestion
Acid Hydrolysis
Enzymatic Digestion
Anaerobic Digestion
Anaerobic Digestion
SIMPLEX/SYLPLEX
(Slagging, Partial Oxidation)
FERTILIZER
FERTILIZER
METHANE
SLUDGE
Partial Combustion
SUGARS
(Chart 8)
LIGNIN
(Chart 8)
SYNTHESIS GAS
(Chart 3)
CARBON MONOXIDE
(Chart 8)

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C.2. Scenario R-2000

The following are specific comments on the charts:

Chart R-2000.1

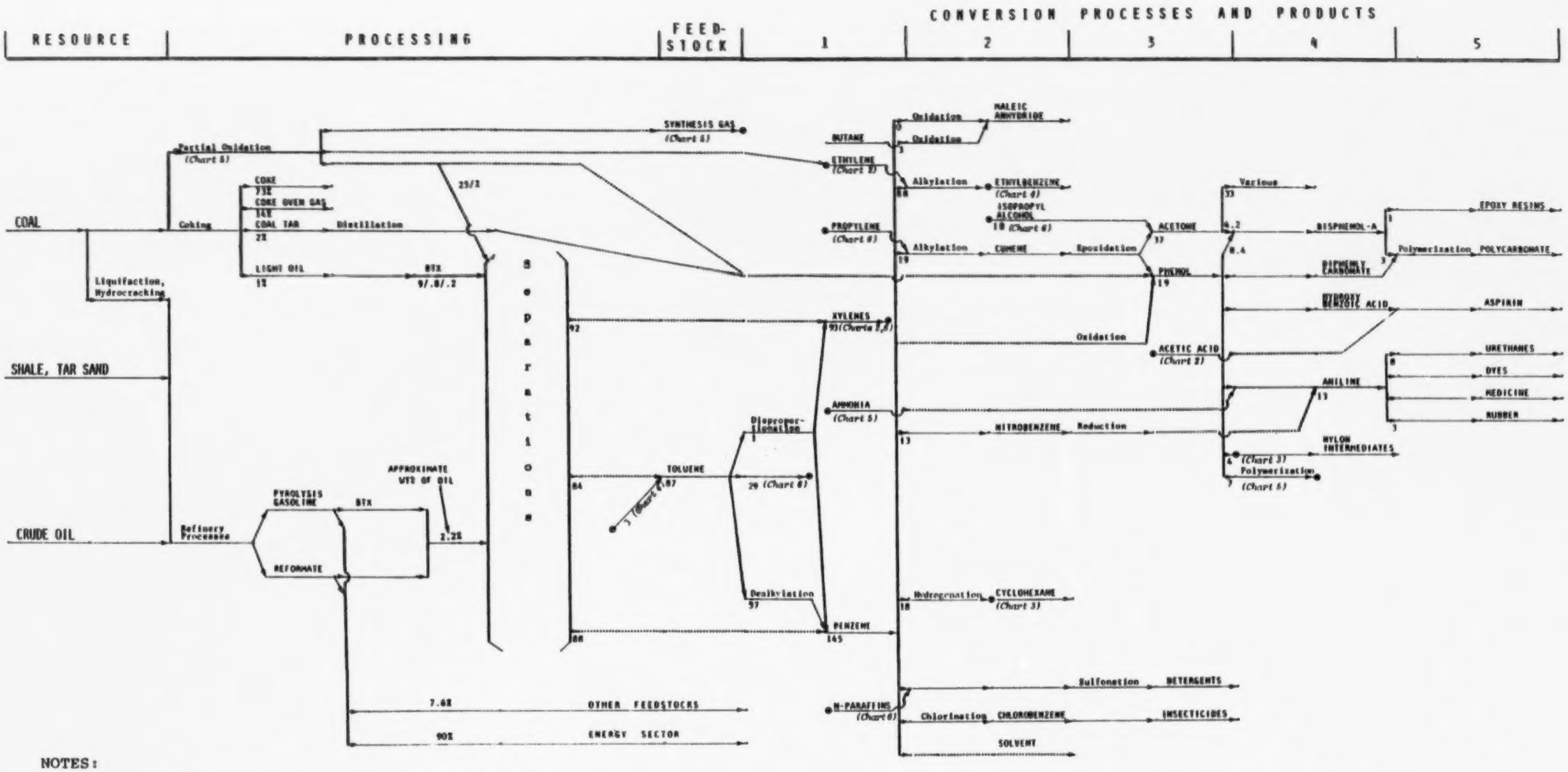
Benzene demand will grow 3.7 percent per year. Polycarbonate polymers are a new growth area but otherwise phenol is weak. Hence, acetone growth will revert to isopropyl alcohol. Maleic anhydride will be lost to butane. Cyclohexane is weak, while aniline is the strongest derivative. Benzene sources are shown on Figure 1 in Section 1.3.6 and Table 7 in Section 1.3.2.

Chart R-2000.2

Ethylene will grow 4.3 percent per year. The major change is that synthesis gas, via methanol and carbonylation chemistry, will capture the acetaldehyde/acetic acid/acetic anhydride market from ethylene, except for the small "other" uses of acetaldehyde (Chart 5), and vinyl acetate (which will show strong growth). Those markets were recently in turn captured by ethylene from acetylene.

Acetylene is a major question. If new processes for cracking residual or crude oil directly to ethylene become common, or if the direct conversion of coal to acetylene by means of an electric arc is commercialized (1, 2) there will be an abundance of acetylene. The most likely uses would be vinyl chloride (now 95 percent from ethylene), and vinyl acetate and butanediol (also via formaldehyde) where major synthesis gas growth is expected. The fastest growth is expected in the small volume E-P (ethylene/propylene) rubber, combined with acrylonitrile and butadiene. The second and third major derivatives of benzene, phenol via cumene and cyclohexane are both used extensively in nylon manufacture, along with, again, acrylonitrile and butadiene. Chart 3 further shows the multiple, overlapping and competitive sources of some chemical intermediates.

SYSTEM R-2000
CHART 1: BENZENE


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL
SHALE, TAR SAND
CRUDE OIL
Partial Oxidation
(Chart 5)
Coking
Liquifaction, Hydrocracking
COKE
73%
COKE OVEN GAS
14%
COAL TAR
2%
Distillation
LIGHT OIL
1%
BTX
9/.8/.2
25/2
Refinery Processes
PYROLYSIS GASOLINE
REFORMATE
BTX
APPROXIMATE WT% OF OIL
2.2%
Separations
7.6%
OTHER FEEDSTOCKS
90%
ENERGY SECTOR
SYNTHESIS GAS
(Chart 5)
92
84
88
TOLUENE
.87
3 (Chart 4)
Disproportionation
1
29 (Chart 8)
Dealkylation
57
BUTANE
ETHYLENE
(Chart 2)
PROPYLENE
(Chart 8)
XYLENES
93 (Charts 2,8)
AMMONIA
(Chart 5)
BENZENE
145
N-PARAFINS
(Chart 6)
Oxidation
Oxidation
3
MALEIC ANHYDRIDE
Alkylation
88
ETHYLBENZENE
(Chart 4)
ISOPROPYL ALCOHOL
10 (Chart 6)
Alkylation
19
CUMENE
Epoxidation
ACETONE
37
PHENOL
19
Oxidation
ACETIC ACID
(Chart 2)
NITROBENZENE
Reduction
13
Hydrogenation
18
CYCLOHEXANE
(Chart 3)
Sulfonation
DETERGENTS
Chlorination
CHLOROBENZENE
INSECTICIDES
SOLVENT
Various
33
4.2
8.4
BISPHENOL-A
DIPHENYL CARBONATE
HYDROXY BENZOIC ACID
ANILINE
11
NYLON INTERMEDIATES
4
(Chart 3)
Polymerization
7
(Chart 5)
1
Polymerization
3
EPOXY RESINS
POLYCARBONATE
ASPIRIN
8
URETHANES
DYES
MEDICINE
RUBBER
3

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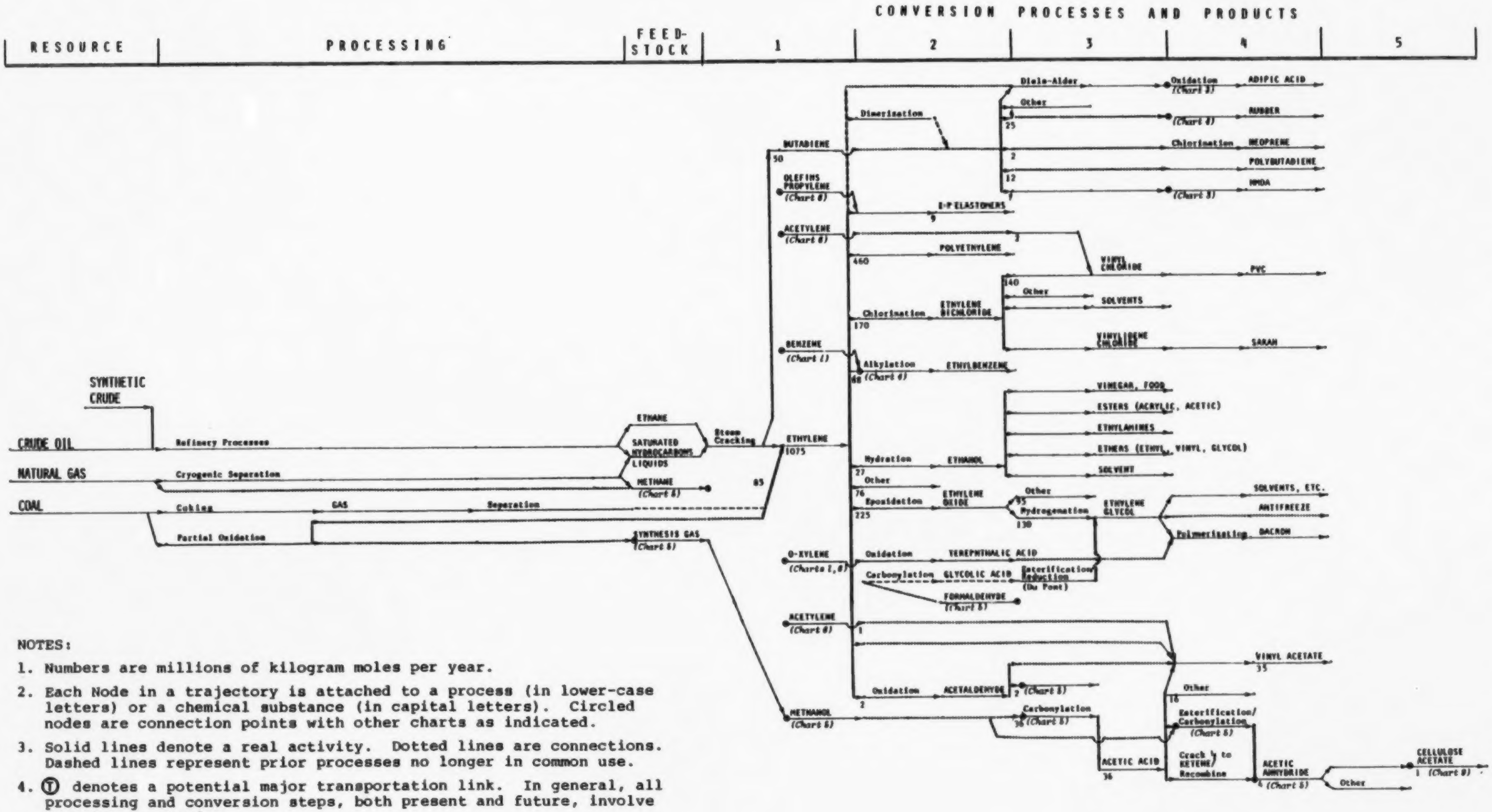
SYSTEM R-2000

CHART 2: ETHYLENE


CONVERSION PROCESSES AND PRODUCTS
RESOURCE
PROCESSING
FEED-STOCK
1
2
3
4
5
SYNTHETIC CRUDE
CRUDE OIL
NATURAL GAS
COAL
Refinery Processes
Cryogenic Separation
Coking
GAS
Separation
Partial Oxidation
ETHANE
SATURATED HYDROCARBONS
LIQUIDS
METHANE (Chart 5)
SYNTHESIS GAS (Chart 5)
Steam Cracking
85
BUTADIENE
50
OLEFINS PROPYLENE (Chart 8)
ACETYLENE (Chart 8)
BENZENE (Chart 1)
ETHYLENE
1075
O-XYLENE (Charts 1,8)
ACETYLENE (Chart 8)
METHANOL (Chart 5)
Dimerization
Diels-Alder
Other
25
2
12
Oxidation (Chart 3)
(Chart 8)
Chlorination
(Chart 3)
ADIPIC ACID
RUBBER
NEOPRENE
POLYBUTADIENE
HMDA
E-P ELASTOMERS
9
POLYETHYLENE
460
VINYL CHLORIDE
PVC
140
Other
SOLVENTS
Chlorination
ETHYLENE DICHLORIDE
170
VINYLIDENE CHLORIDE
SARAN
Alkylation (Chart 6)
68
ETHYLBENZENE
VINEGAR, FOOD
ESTERS (ACRYLIC, ACETIC)
ETHYLAMINES
ETHERS (ETHYL, VINYL, GLYCOL)
SOLVENT
Hydration
ETHANOL
27
Other
76
Epoxidation
ETHYLENE OXIDE
225
Other
95
Hydrogenation
130
ETHYLENE GLYCOL
SOLVENTS, ETC.
ANTIFREEZE
Polymerizating
DACRON
Oxidation
TEREPHTHALIC ACID
Carbonylation
GLYCOLIC ACID
Esterification Reduction (Du Pont)
FORMALDEHYDE (Chart 5)
1
VINYL ACETATE
35
Oxidation
ACETALDEHYDE
2
2 (Chart 5)
Carbonylation
36 (Chart 5)
Other
16
Esterification/Carbonylation (Chart 5)
ACETIC ACID
36
Crack ½ to KETENE/Recombine
ACETIC ANHYDRIDE
4 (Chart 5)
Other
CELLULOSE ACETATE
1 (Chart 9)

NOTES:

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2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
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4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

elastomers. Ethylene sources are shown in Figure 2, Section 1.3.6 and Table 7, Section 1.3.2.

Chart R-2000.3

Cyclohexane will grow two percent per year. A major recent change is loss of its sole-source status for Nylon 6,6. As the ethylene source shifts from gas to oil and from light hydrocarbons to naphtha, butadiene and acrylonitrile (from propylene) will be increasingly plentiful and competitive.

Chart R-2000.4

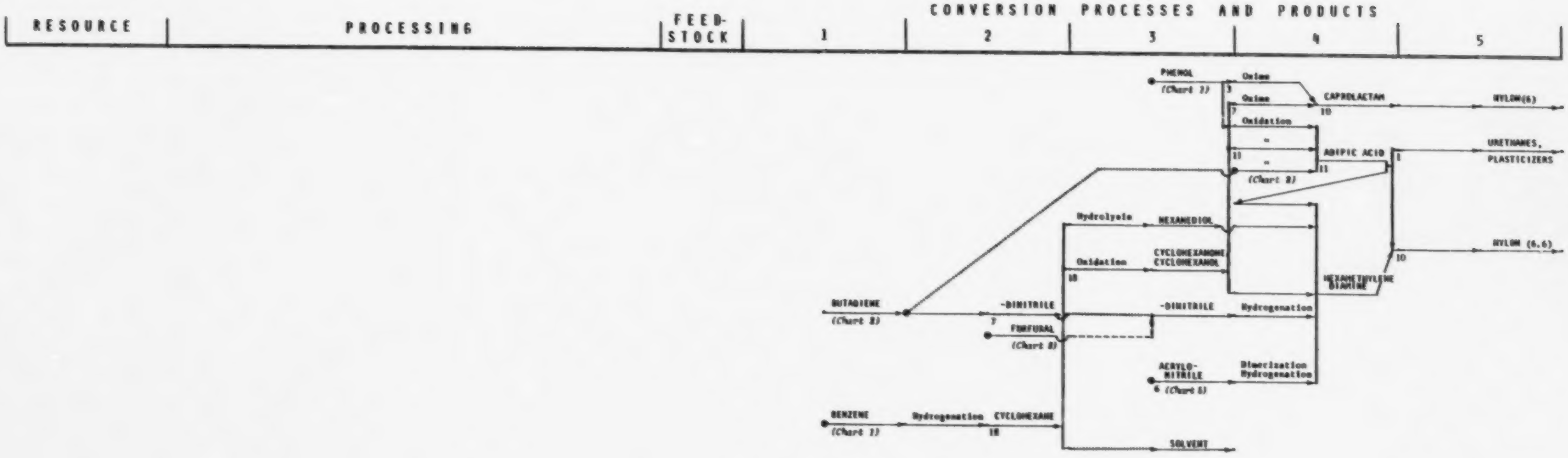
Ethylbenzene and styrene will grow five percent per year. These chemicals are closely tied; virtually all ethylbenzene goes into styrene in combined plants. Their growth will be led by copolymers with acrylonitrile and butadiene.

Chart R-2000.5

Synthesis Gas (CO/H_2) will grow four percent per year. Coal will capture all new demand - 55 percent of the total capacity by 2000. The major strength is carbonylation chemistry capture of the acetic acid group. The major uncertainty is the status of formaldehyde as a possible carcinogen. Formaldehyde is used in the manufacture of urea-formaldehyde insulation and phenol-formaldehyde adhesives (plywood and particle board). The foam insulation industry has collapsed during the controversy (3). Butanediol could become the prinicipal formaldehyde use. The manufacture of animal feed and fertilizer will continue to dominate the synthesis gas uses, although perhaps using only 70 percent rather than 85 percent overall.

SYSTEM R-2000

CHART 3: CYCLOHEXANE


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
PHENOL
(Chart 1)
3
Oxime
Oxime
7
CAPROLACTAM
10
NYLON(6)
Oxidation
"
11
"
ADIPIC ACID
11
(Chart 8)
1
URETHANES,
PLASTICIZERS
Hydrolysis
HEXANEDIOL
Oxidation
10
CYCLOHEXANONE,
CYCLOHEXANOL
NYLON (6,6)
10
HEXAMETHYLENE DIAMINE
BUTADIENE
(Chart 8)
-DINITRILE
7
FURFURAL
(Chart 8)
-DINITRILE
Hydrogenation
ACRYLO-
NITRILE
6 (Chart 5)
Dimerization
Hydrogenation
BENZENE
(Chart 1)
Hydrogenation
CYCLOHEXANE
18
SOLVENT

NOTES:

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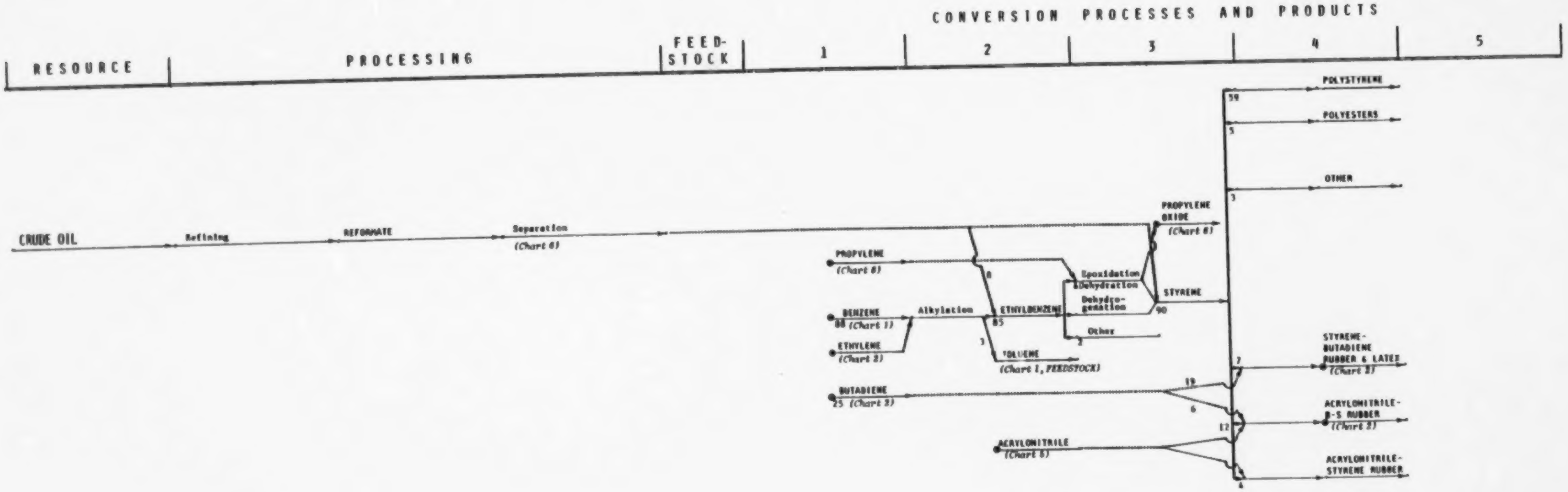
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM R-2000

CHART 4: ETHYLBENZENE, STYRENE

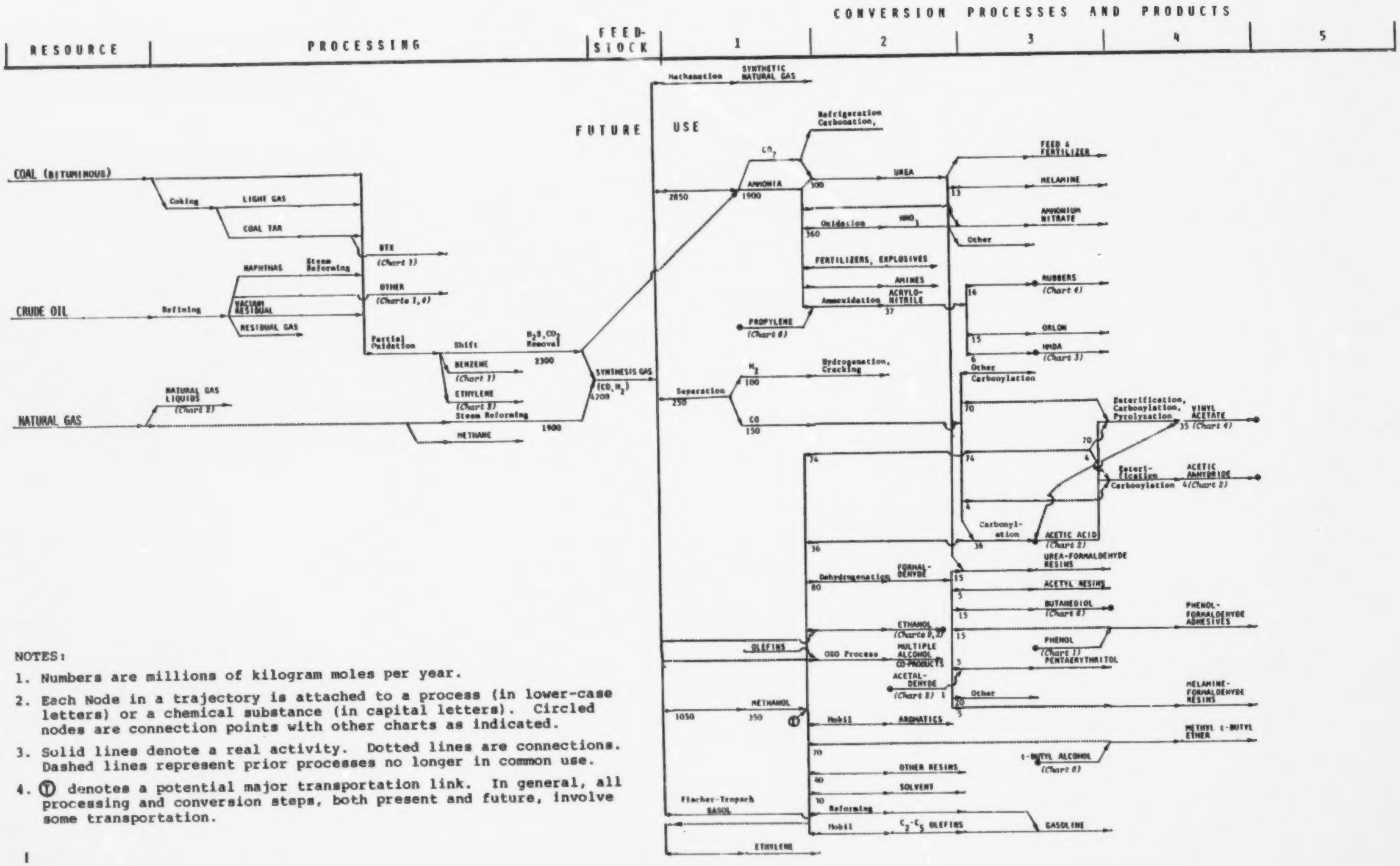

CONVERSION PROCESSES AND PRODUCTS
RESOURCE
PROCESSING
FEED-STOCK
1
2
3
4
5
CRUDE OIL
Refining
REFORMATE
Separation
(Chart 8)
PROPYLENE
(Chart 8)
BENZENE
88 (Chart 1)
ETHYLENE
(Chart 2)
Alkylation
8
ETHYLBENZENE
85
3
TOLUENE
(Chart 1, FEEDSTOCK)
Epoxidation
Dehydration
Dehydro-genation
Other
2
PROPYLENE OXIDE
(Chart 8)
STYRENE
90
BUTADIENE
25 (Chart 2)
19
6
ACRYLONITRILE
(Chart 5)
59
POLYSTYRENE
5
POLYESTERS
3
OTHER
7
STYRENE-BUTADIENE RUBBER & LATEX
(Chart 2)
12
ACRYLONITRILE-B-S RUBBER
(Chart 2)
4
ACRYLONITRILE-STYRENE RUBBER

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM R-2000

CHART 5: SYNTHESIS GAS


CONVERSION PROCESSES AND PRODUCTS
RESOURCE
PROCESSING
FEED-STOCK
1
2
3
4
5
FUTURE USE
COAL (BITUMINOUS)
Coking
LIGHT GAS
COAL TAR
BTX
(Chart 1)
NAPHTHAS
Steam Reforming
OTHER
(Charts 1,4)
CRUDE OIL
Refining
VACUUM RESIDUAL
RESIDUAL GAS
Partial Oxidation
Shift
H_2S, CO_2 Removal
2300
BENZENE
(Chart 1)
ETHYLENE
(Chart 8)
Steam Reforming
1900
METHANE
NATURAL GAS LIQUIDS
(Chart 8)
NATURAL GAS
SYNTHESIS GAS
(CO, H_2)
4200
Methanation
SYNTHETIC NATURAL GAS
Refrigeration Carbonation,
CO_2
AMMONIA
2850
1900
100
UREA
FEED & FERTILIZER
MELAMINE
13
Oxidation
HNO_3
360
AMMONIUM NITRATE
Other
FERTILIZERS, EXPLOSIVES
AMINES
Ammoxidation
ACRYLO-NITRILE
37
PROPYLENE
(Chart 8)
RUBBERS
(Chart 4)
16
ORLON
15
HMDA
(Chart 3)
6
Other Carbonylation
Separation
250
H_2
100
Hydrogenation, Cracking
CO
150
70
Esterification, Carbonylation, Pyrolyzation
VINYL ACETATE
35 (Chart 4)
70
74
74
4
Esteri-fication
Carbonylation
ACETIC ANHYDRIDE
4 (Chart 2)
4
Carbonyl-ation
ACETIC ACID
(Chart 2)
36
36
UREA-FORMALDEHYDE RESINS
Dehydrogenation
FORMAL-DEHYDE
80
15
ACETYL RESINS
5
BUTANEDIOL
(Chart 8)
15
PHENOL-FORMALDEHYDE ADHESIVES
ETHANOL
(Charts 8,2)
15
PHENOL
(Chart 1)
OLEFINS
OXO Process
MULTIPLE ALCOHOL CO-PRODUCTS
5
PENTAERYTHRITOL
ACETAL-DEHYDE
(Chart 8)
1
Other
20
MELAMINE-FORMALDEHYDE RESINS
METHANOL
1050
350
Ⓣ
Mobil
AROMATICS
5
METHYL t-BUTYL ETHER
70
t-BUTYL ALCOHOL
(Chart 8)
OTHER RESINS
40
SOLVENT
Fischer-Tropsch SASOL
30
Reforming
GASOLINE
Mobil
C_2-C_5 OLEFINS
ETHYLENE

NOTES:

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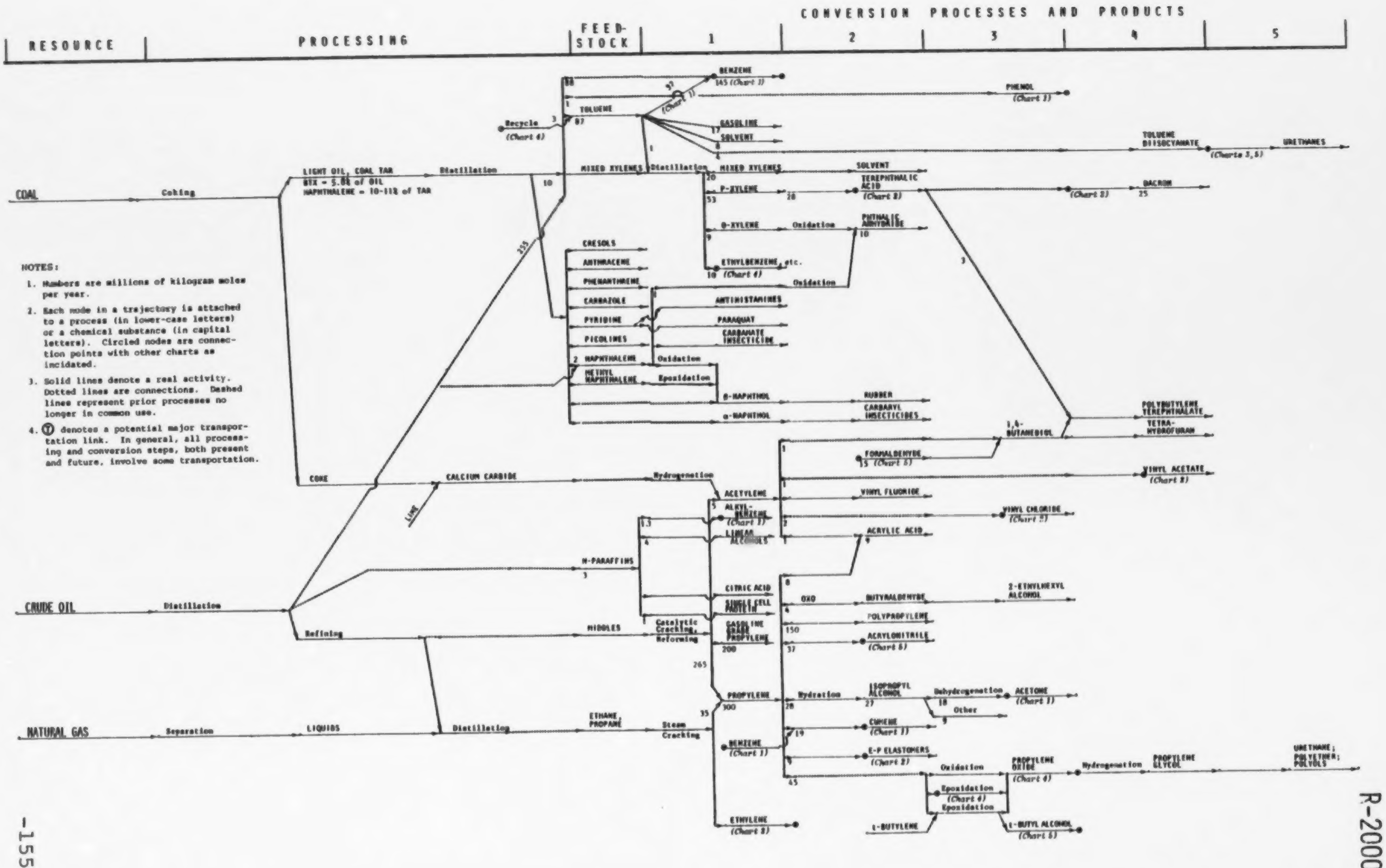
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

Chart R-2000.6

Toluene production will grow 3.5 percent per year. Xylene will grow 4.2 percent per year, led in the near term by new terephthalic acid uses PET and PBT. Paraffins will grow about two percent per year, but their use in single-cell protein cultures could mushroom. Naphthalene will grow about one percent per year. Acetylene could change plus or minus ten percent per year. It could continue its long term slide or be reinvigorated, as discussed in the R-2000.2 notes. Propylene will grow 3.5 percent per year, led by continuing high growth of polypropylene.

SYSTEM R-2000

CHART 6: OTHER BASIC CHEMICALS


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL
Coking
LIGHT OIL, COAL TAR
BTX = 5.8% of OIL
NAPHTHALENE = 10-11% of TAR
Distillation
10
255
Recycle
(Chart 4)
3
88
1
TOLUENE
87
97
(Chart 1)
BENZENE
145 (Chart 1)
PHENOL
(Chart 1)
GASOLINE
17
SOLVENT
8
4
1
TOLUENE DIISOCYANATE
(Charts 3,5)
URETHANES
MIXED XYLENES
Distillation
MIXED XYLENES
20
SOLVENT
P-XYLENE
53
28
TEREPHTHALIC ACID
(Chart 8)
(Chart 2)
DACRON
25
O-XYLENE
9
Oxidation
PHTHALIC ANHYDRIDE
10
ETHYLBENZENE, etc.
10 (Chart 4)
Oxidation
3
CRESOLS
ANTHRACENE
PHENANTHRENE
CARBAZOLE
PYRIDINE
PICOLINES
2 NAPHTHALENE
METHYL NAPHTHALENE
Oxidation
Epoxidation
ANTIHISTAMINES
PARAQUAT
CARBAMATE INSECTICIDE
β-NAPHTHOL
α-NAPHTHOL
RUBBER
CARBARYL INSECTICIDES
1,4-BUTANEDIOL
POLYBUTYLENE TEREPHTHALATE
TETRA-HYDROFURAN
COKE
CALCIUM CARBIDE
LIME
Hydrogenation
ACETYLENE
1
FORMALDEHYDE
15 (Chart 5)
1
VINYL ACETATE
(Chart 8)
VINYL FLUORIDE
2
VINYL CHLORIDE
(Chart 2)
1
ACRYLIC ACID
9
5
ALKYL-BENZENE
(Chart 1)
1.3
LINEAR ALCOHOLS
4
N-PARAFFINS
3
CITRIC ACID
SINGLE CELL PROTEIN
GASOLINE GRADE PROPYLENE
200
CRUDE OIL
Distillation
Refining
MIDDLES
Catalytic Cracking, Reforming
265
8
OXO
BUTYRALDEHYDE
2-ETHYLHEXYL ALCOHOL
4
POLYPROPYLENE
150
ACRYLONITRILE
37
(Chart 6)
PROPYLENE
300
Hydration
28
ISOPROPYL ALCOHOL
27
Dehydrogenation
18
ACETONE
(Chart 1)
Other
9
35
NATURAL GAS
Separation
LIQUIDS
Distillation
ETHANE, PROPANE
Steam Cracking
BENZENE
(Chart 1)
19
CUMENE
(Chart 1)
E-P ELASTOMERS
(Chart 2)
45
Oxidation
PROPYLENE OXIDE
(Chart 4)
Hydrogenation
PROPYLENE GLYCOL
URETHANE; POLYETHER; POLYOLS
Epoxidation
(Chart 4)
Epoxidation
t-BUTYLENE
t-BUTYL ALCOHOL
(Chart 5)
ETHYLENE
(Chart 8)

NOTES:

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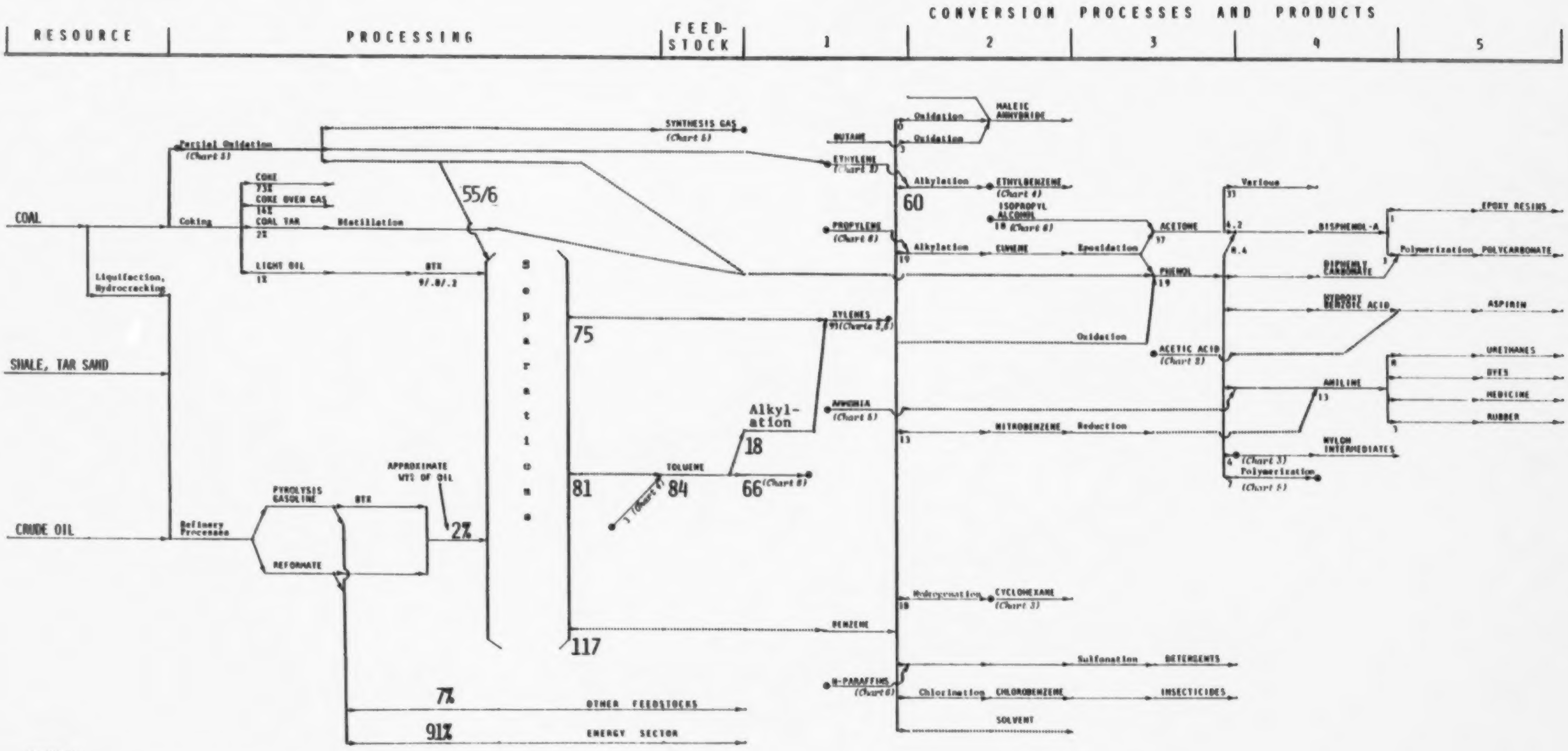
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

C.3. Scenario A-1: Synthesis Gas

Changes in the basic chemical system are shown in larger type in the Reference Materials System A-1 Charts 1, 2, 4, 5, and 6. The contributions of synthesis gas to total feedstocks and to the key chemicals are summarized in Table 7, Section 1.3.3. There is also the potential for producing longer chain olefins, via the OXO, Mobil or Fischer-Tropsch processes (2), but that does not directly affect the basic chemicals. This reference also discusses methanol and ammonia production economics.

SYSTEM A-1: SYNTHESIS GAS

CHART 1: BENZENE


CONVERSION PROCESSES AND PRODUCTS
RESOURCE
PROCESSING
FEED-STOCK
1
2
3
4
5
COAL
SHALE, TAR SAND
CRUDE OIL
Partial Oxidation (Chart 5)
Coking
Liquifaction, Hydrocracking
Refinery Processes
COKE 73%
COKE OVEN GAS 14%
COAL TAR 2%
LIGHT OIL 1%
Distillation
BTX 9/.8/.2
55/6
PYROLYSIS GASOLINE
REFORMATE
BTX
APPROXIMATE WT% OF OIL
2%
7%
OTHER FEEDSTOCKS
91%
ENERGY SECTOR
Separations
75
81
117
SYNTHESIS GAS (Chart 5)
TOLUENE
84
3 (Chart 8)
Alkyl-ation
18
66 (Chart 8)
BUTANE
ETHYLENE (Chart 3)
PROPYLENE (Chart 8)
XYLENES 91 (Charts 5,8)
AMMONIA (Chart 5)
BENZENE
N-PARAFFINS (Chart 6)
Oxidation
Oxidation
MALEIC ANHYDRIDE
6
3
Alkylation
60
ETHYLBENZENE (Chart 4)
ISOPROPYL ALCOHOL
18 (Chart 6)
Alkylation
19
CUMENE
Epoxidation
ACETONE
37
PHENOL
19
Oxidation
ACETIC ACID (Chart 8)
NITROBENZENE
Reduction
13
Hydrogenation
CYCLOHEXANE (Chart 3)
18
Sulfonation
DETERGENTS
Chlorination
CHLOROBENZENE
INSECTICIDES
SOLVENT
Various
33
4.2
8.4
BISPHENOL-A
DIPHENYL CARBONATE
HYDROXY BENZOIC ACID
ANILINE
13
NYLON INTERMEDIATES
4 (Chart 3)
Polymerization
7 (Chart 5)
1
EPOXY RESINS
Polymerization
POLYCARBONATE
3
ASPIRIN
8
URETHANES
DYES
MEDICINE
RUBBER
3

NOTES:

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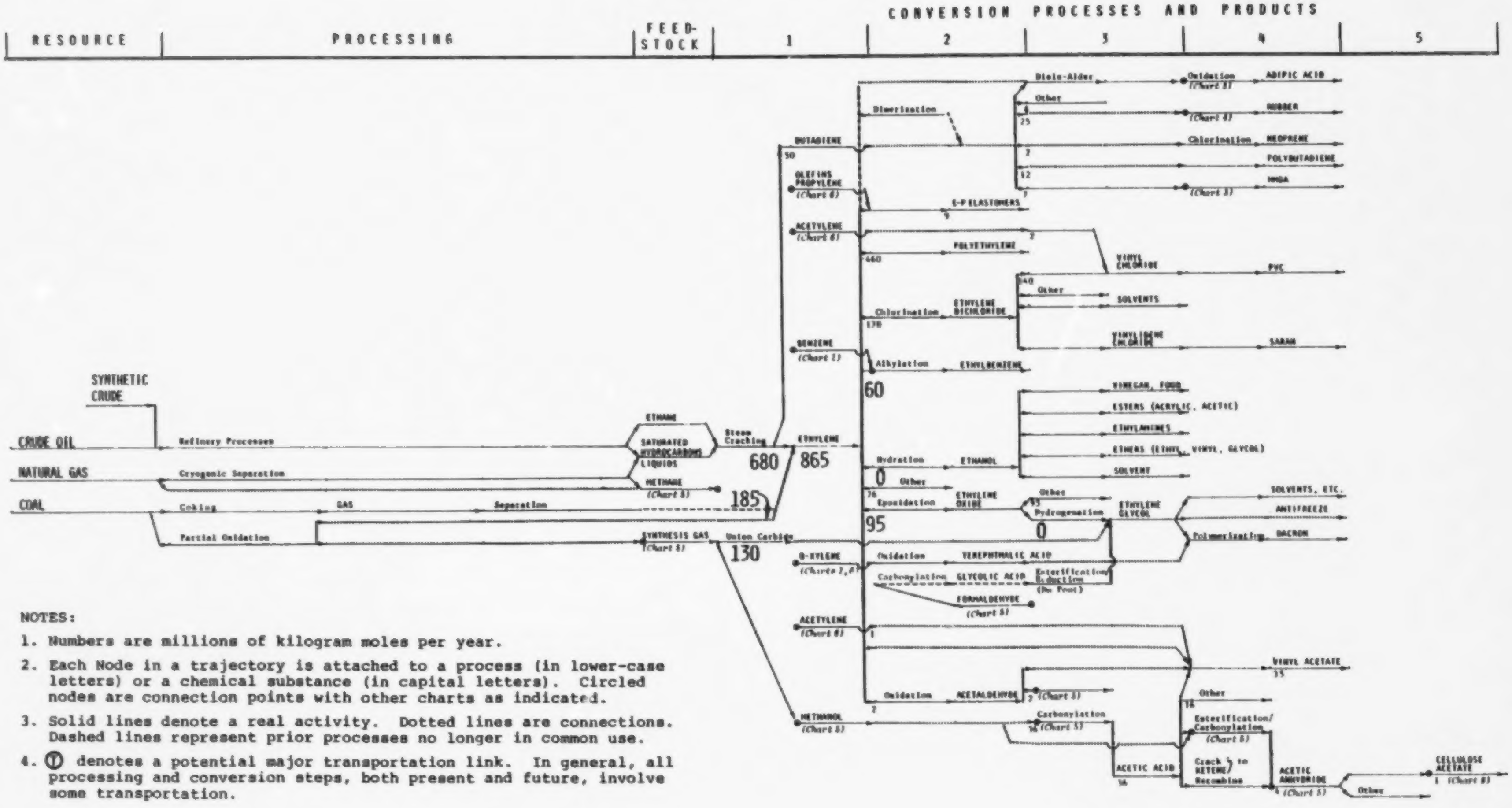
SYSTEM A-1: SYNTHESIS GAS

CHART 2: ETHYLENE



RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
SYNTHETIC CRUDE
CRUDE OIL
NATURAL GAS
COAL
Refinery Processes
Cryogenic Separation
Coking
GAS
Separation
Partial Oxidation
ETHANE
SATURATED HYDROCARBONS
LIQUIDS
METHANE (Chart 5)
SYNTHESIS GAS (Chart 5)
Steam Cracking
680
185
Union Carbide
130
ETHYLENE
865
BUTADIENE
50
OLEFINS PROPYLENE (Chart 6)
ACETYLENE (Chart 6)
BENZENE (Chart 1)
O-XYLENE (Charts 1,6)
ACETYLENE (Chart 6)
METHANOL (Chart 5)
Diels-Alder
Dimerization
Other
25
Oxidation (Chart 3)
ADIPIC ACID
(Chart 4)
RUBBER
Chlorination
NEOPRENE
2
POLYBUTADIENE
12
7
(Chart 3)
HMDA
E-P ELASTOMERS
9
2
POLYETHYLENE
460
VINYL CHLORIDE
PVC
140
Other
SOLVENTS
Chlorination
ETHYLENE DICHLORIDE
170
VINYLIDENE CHLORIDE
SARAN
Alkylation
ETHYLBENZENE
60
VINEGAR, FOOD
ESTERS (ACRYLIC, ACETIC)
ETHYLAMINES
ETHERS (ETHYL, VINYL, GLYCOL)
SOLVENT
Hydration
ETHANOL
0
Other
76
Epoxidation
ETHYLENE OXIDE
95
Other
55
Hydrogenation
0
ETHYLENE GLYCOL
SOLVENTS, ETC.
ANTIFREEZE
Polymerization
DACRON
Oxidation
TEREPHTHALIC ACID
Carbonylation
GLYCOLIC ACID
Esterification Reduction (Du Pont)
FORMALDEHYDE (Chart 5)
1
VINYL ACETATE
35
Oxidation
ACETALDEHYDE
2
2 (Chart 3)
Carbonylation
16 (Chart 5)
Other
16
Esterification/ Carbonylation (Chart 5)
ACETIC ACID
16
Crack ½ to KETENE/ Recombine
ACETIC ANHYDRIDE
4 (Chart 5)
Other
CELLULOSE ACETATE
1 (Chart 8)

NOTES:

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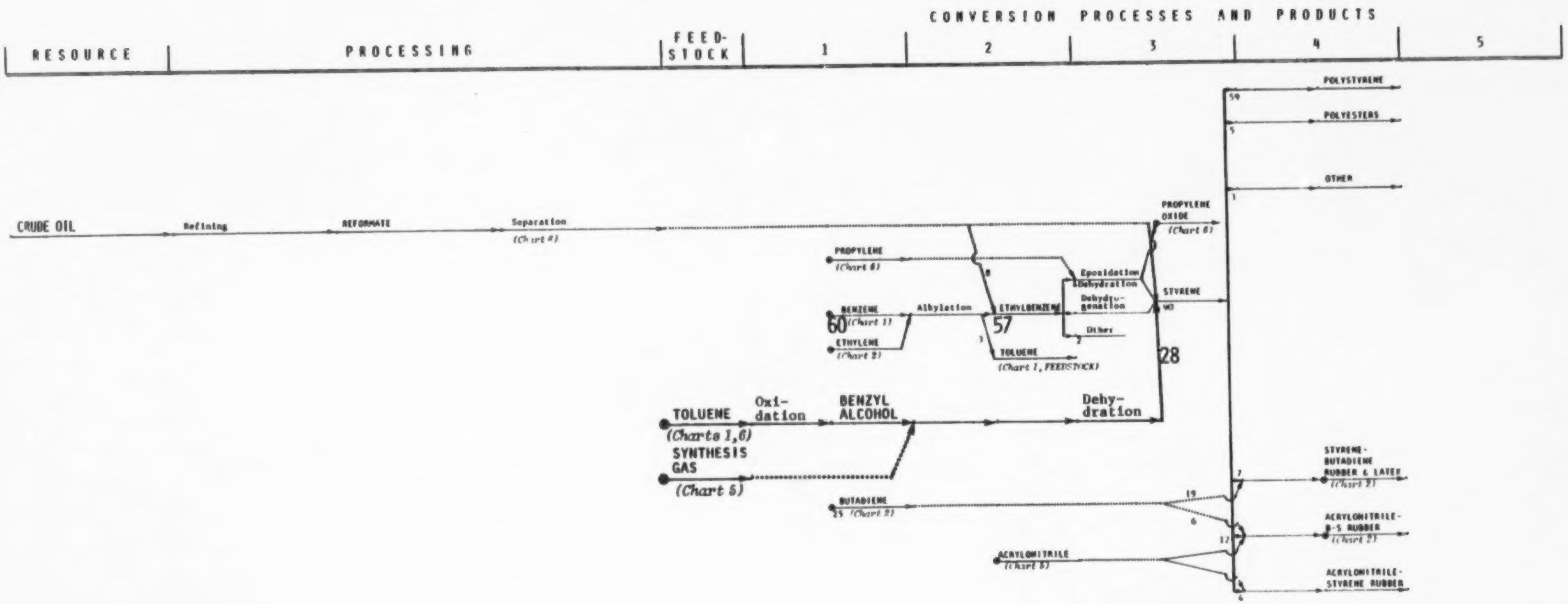
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-1: SYNTHESIS GAS

CHART 4: ETHYLBENZENE, STYRENE

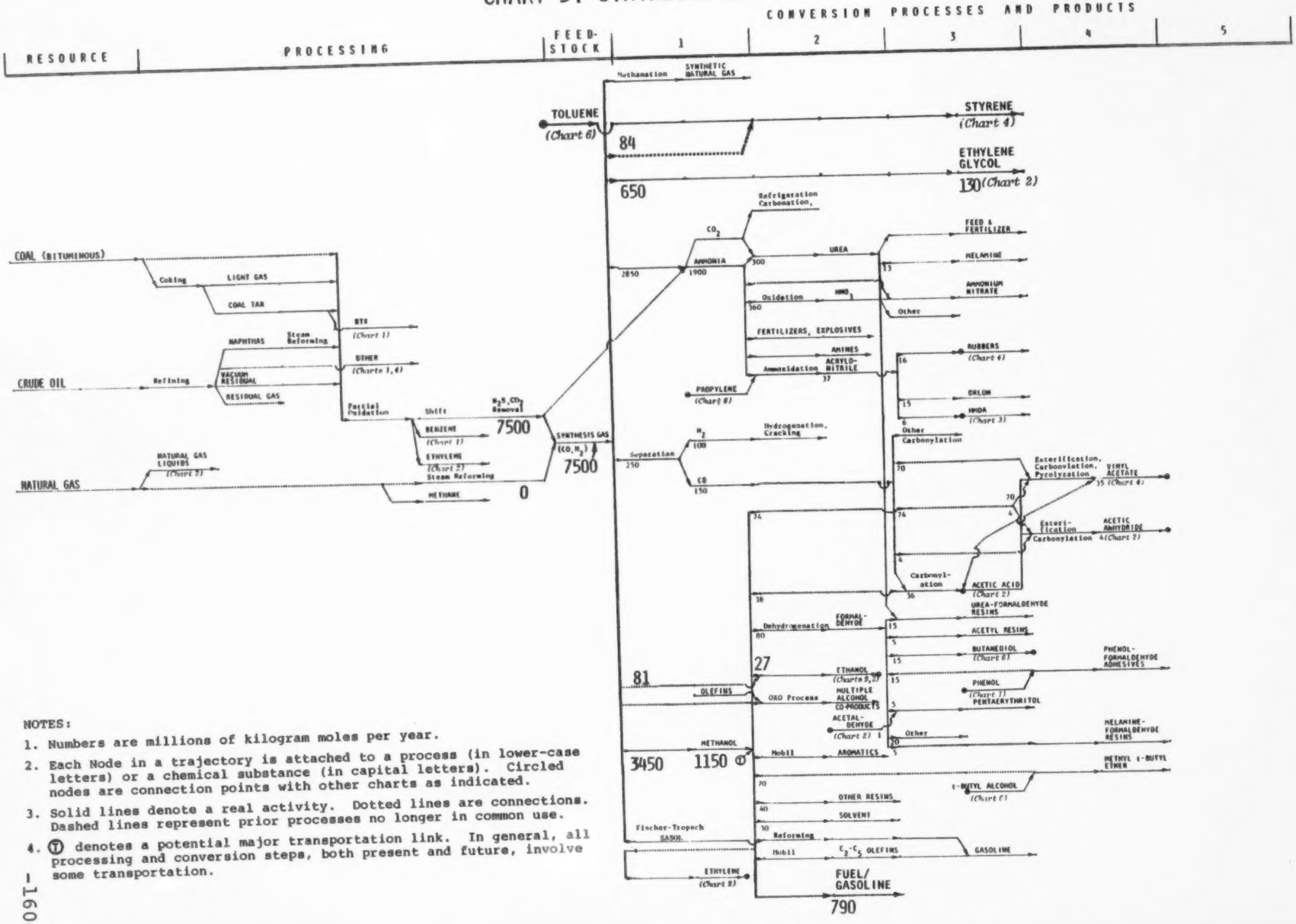

RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
CRUDE OIL
Refining
REFORMATE
Separation
PROPYLENE
(Chart 6)
BENZENE
60
(Chart 1)
ETHYLENE
(Chart 2)
Alkylation
8
ETHYLBENZENE
57
3
TOLUENE
(Chart 1, FEEDSTOCK)
Epoxidation
Dehydration
Dehydro-genation
Other
2
PROPYLENE OXIDE
(Chart 6)
STYRENE
28
TOLUENE
(Charts 1,6)
Oxi-dation
BENZYL ALCOHOL
Dehy-dration
SYNTHESIS GAS
(Chart 5)
BUTADIENE
25
(Chart 2)
ACRYLONITRILE
(Chart 3)
19
6
59
POLYSTYRENE
5
POLYESTERS
1
OTHER
7
STYRENE-BUTADIENE RUBBER & LATEX
(Chart 2)
12
ACRYLONITRILE-B-S RUBBER
(Chart 2)
4
ACRYLONITRILE-STYRENE RUBBER

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-1: SYNTHESIS GAS

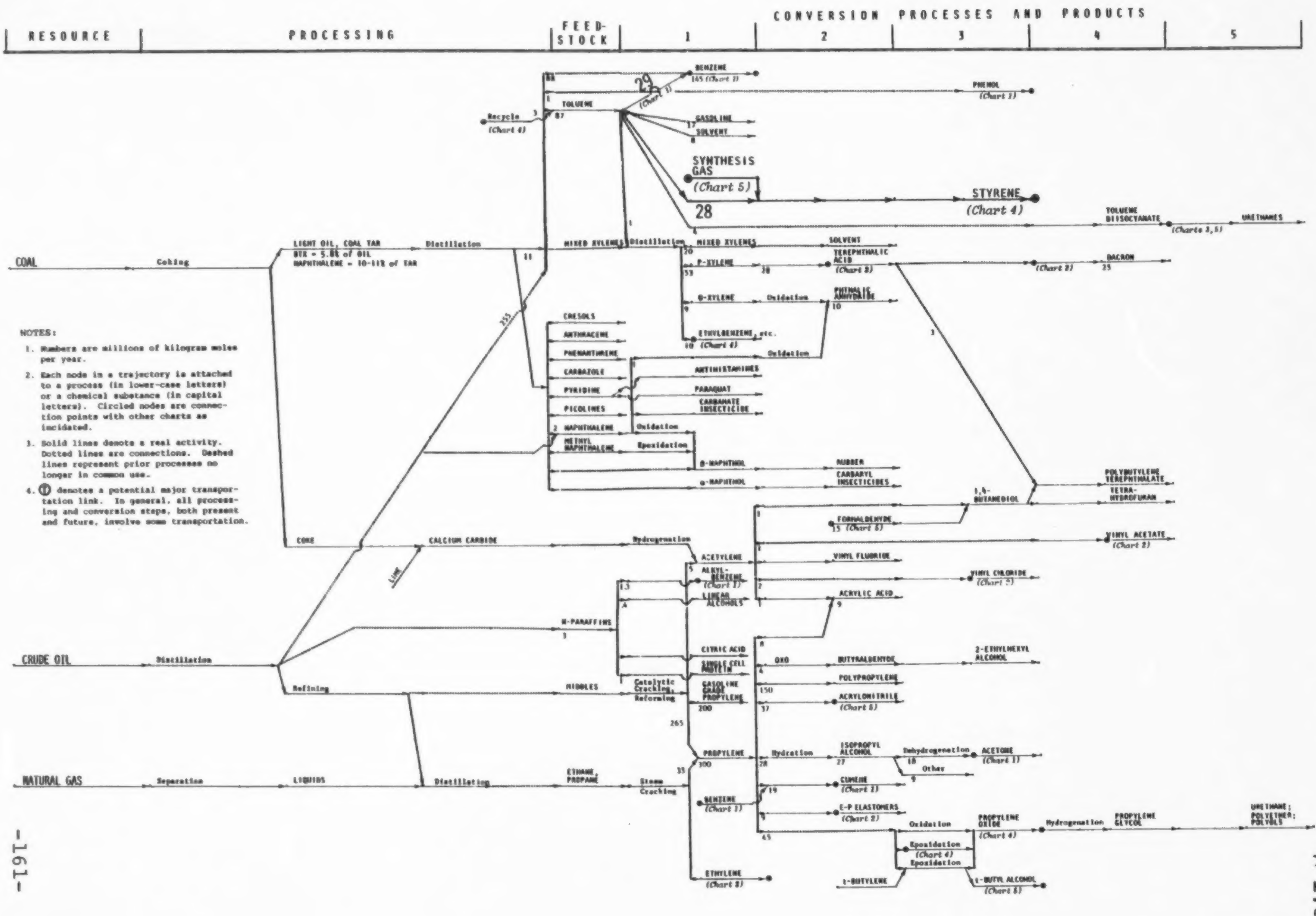
CHART 5: SYNTHESIS GAS


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL (BITUMINOUS)
Coking
LIGHT GAS
COAL TAR
CRUDE OIL
Refining
NAPHTHAS
Steam Reforming
VACUUM RESIDUAL
RESIDUAL GAS
BTX
(Chart 1)
OTHER
(Charts 1,4)
NATURAL GAS
NATURAL GAS LIQUIDS
(Chart 2)
Partial Oxidation
Shift
H_2S, CO_2 Removal
7500
BENZENE
(Chart 1)
ETHYLENE
(Chart 2)
Steam Reforming
METHANE
0
SYNTHESIS GAS
(CO, H_2)
7500
TOLUENE
(Chart 6)
Methanation
SYNTHETIC NATURAL GAS
84
STYRENE
(Chart 4)
650
ETHYLENE GLYCOL
130 (Chart 2)
Refrigeration Carbonation,
CO_2
AMMONIA
2850
1900
300
UREA
FEED & FERTILIZER
MELAMINE
13
Oxidation
360
HNO_3
AMMONIUM NITRATE
Other
FERTILIZERS, EXPLOSIVES
AMINES
Ammoxidation
ACRYLO-NITRILE
37
PROPYLENE
(Chart 8)
16
RUBBERS
(Chart 4)
15
ORLON
6
HMDA
(Chart 3)
Separation
250
H_2
100
Hydrogenation, Cracking
CO
150
Other Carbonylation
70
Esterification, Carbonylation, Pyrolyzation
VINYL ACETATE
35 (Chart 4)
70
74
74
4
Esteri-fication
Carbonylation
ACETIC ANHYDRIDE
4 (Chart 2)
4
Carbonyl-ation
36
ACETIC ACID
(Chart 2)
38
UREA-FORMALDEHYDE RESINS
Dehydrogenation
80
FORMAL-DEHYDE
15
ACETYL RESINS
5
BUTANEDIOL
(Chart 8)
15
27
81
OLEFINS
ETHANOL
(Charts 9,2)
15
PHENOL-FORMALDEHYDE ADHESIVES
PHENOL
(Chart 1)
OXO Process
MULTIPLE ALCOHOL CO-PRODUCTS
5
PENTAERYTHRITOL
ACETAL-DEHYDE
(Chart 2) 1
Other
20
MELAMINE-FORMALDEHYDE RESINS
METHANOL
3450
1150 Ⓣ
Mobil
AROMATICS
5
METHYL t-BUTYL ETHER
70
t-BUTYL ALCOHOL
(Chart C)
OTHER RESINS
40
SOLVENT
30
Fischer-Tropsch SASOL
Reforming
Mobil
C_2-C_5 OLEFINS
GASOLINE
ETHYLENE
(Chart 8)
FUEL/ GASOLINE
790

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-1: SYNTHESIS GAS
CHART 6: OTHER BASIC CHEMICALS


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL
Coking
LIGHT OIL, COAL TAR
BTX = 5.8% of OIL
NAPHTHALENE = 10-11% of TAR
Distillation
11
255
MIXED XYLENES
Distillation
88
1
TOLUENE
3
87
Recycle
(Chart 4)
BENZENE
145 (Chart 1)
29
(Chart 1)
PHENOL
(Chart 1)
17
GASOLINE
8
SOLVENT
SYNTHESIS GAS
(Chart 5)
28
STYRENE
(Chart 4)
4
TOLUENE DIISOCYANATE
(Charts 3,5)
URETHANES
1
MIXED XYLENES
20
SOLVENT
P-XYLENE
53
28
TEREPHTHALIC ACID
(Chart 2)
(Chart 2)
DACRON
25
O-XYLENE
9
Oxidation
PHTHALIC ANHYDRIDE
10
ETHYLBENZENE, etc.
10 (Chart 4)
Oxidation
3
CRESOLS
ANTHRACENE
PHENANTHRENE
CARBAZOLE
PYRIDINE
PICOLINES
2 NAPHTHALENE
METHYL NAPHTHALENE
1
ANTIHISTAMINES
PARAQUAT
CARBAMATE INSECTICIDE
Oxidation
Epoxidation
β-NAPHTHOL
RUBBER
α-NAPHTHOL
CARBARYL INSECTICIDES
1,4-BUTANEDIOL
POLYBUTYLENE TEREPHTHALATE
TETRA-HYDROFURAN
CRUDE OIL
Distillation
COKE
CALCIUM CARBIDE
LIME
Hydrogenation
ACETYLENE
5
ALKYL-BENZENE
(Chart 1)
13
LINEAR ALCOHOLS
4
3
FORMALDEHYDE
15 (Chart 5)
1
VINYL ACETATE
(Chart 2)
VINYL FLUORIDE
2
VINYL CHLORIDE
(Chart 2)
1
ACRYLIC ACID
9
N-PARAFFINS
1
CITRIC ACID
SINGLE CELL PROTEIN
Refining
MIDDLES
Catalytic Cracking, Reforming
1
GASOLINE GRADE PROPYLENE
200
265
8
OXO
4
BUTYRALDEHYDE
2-ETHYLHEXYL ALCOHOL
POLYPROPYLENE
150
ACRYLONITRILE
37
(Chart 5)
PROPYLENE
300
Hydration
28
ISOPROPYL ALCOHOL
27
Dehydrogenation
18
ACETONE
(Chart 1)
Other
9
NATURAL GAS
Separation
LIQUIDS
Distilling
ETHANE, PROPANE
Steam Cracking
35
BENZENE
(Chart 1)
19
CUMENE
(Chart 1)
9
E-P ELASTOMERS
(Chart 2)
45
Oxidation
PROPYLENE OXIDE
(Chart 4)
Hydrogenation
PROPYLENE GLYCOL
URETHANE; POLYETHER; POLYOLS
Epoxidation
(Chart 4)
Epoxidation
t-BUTYLENE
t-BUTYL ALCOHOL
(Chart 5)
ETHYLENE
(Chart 2)

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as incidated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

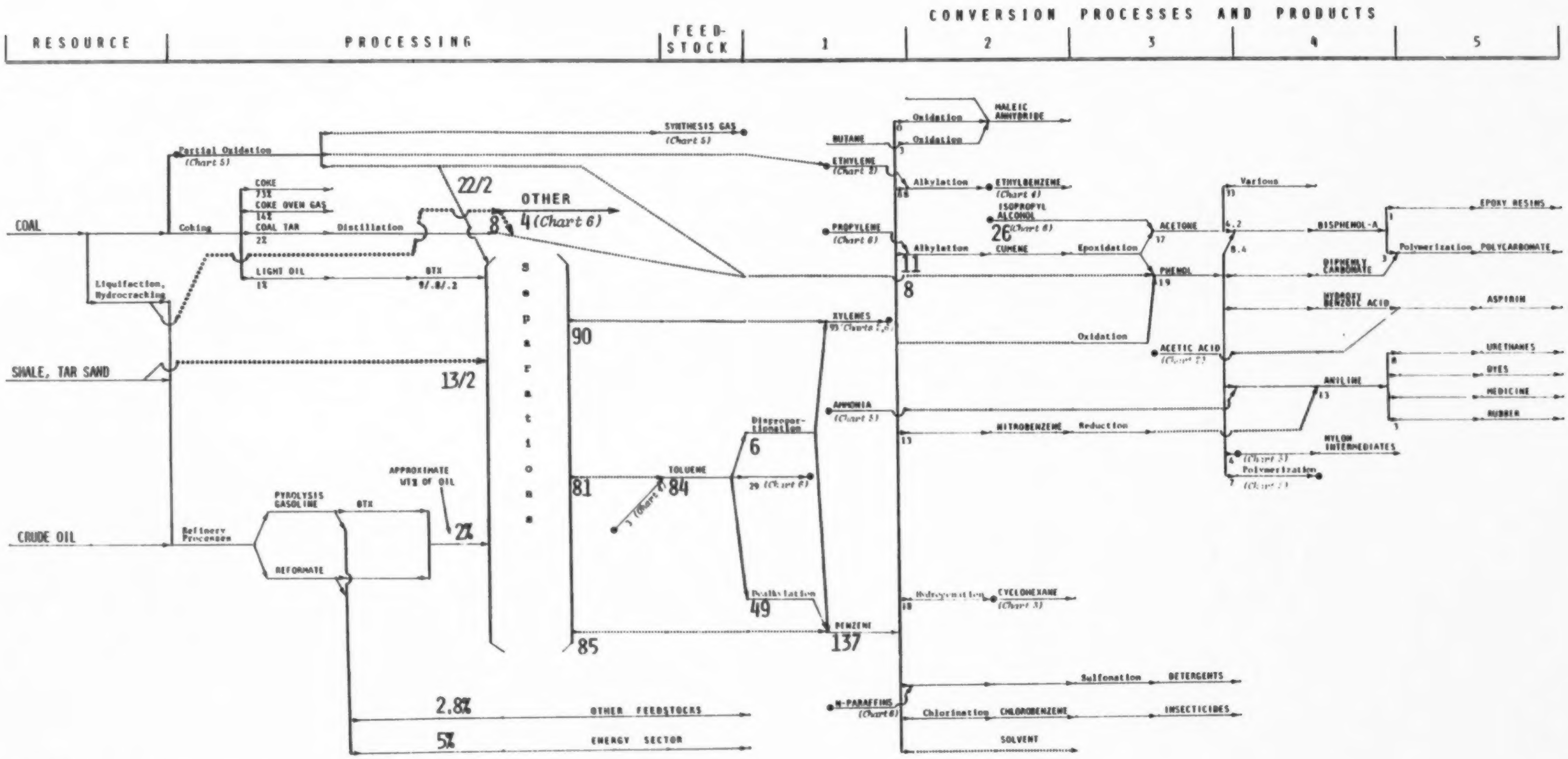
C.4. Scenario A-2: Synfuel By-Products

The outcome of the development of a major synfuel industry is shown on the Reference Material System A-2 Charts 1, 2, 5, 6, 7, and 8. Phenol, on Chart A-2.1 produced from coal hydrocracking has a multi-step impact. Less phenol is produced by epoxidation so less propylene and benzene are required. But also less acetone is produced, so that propylene is diverted to making isopropyl alcohol on A-2.6.

On Chart A-2.2, only a new supply of saturated hydrocarbons for cracking appears. Coal and shale on Chart A-2.5 supply methane for synthesis gas but also have an ammonia by-product which decreases syngas demand. Chart A-2.6 displays the naphthalene produced from synfuels plants. Charts A-2.7 and 8 show the complete coal- and shale-based chemical trees which connect into the prior charts.

SYSTEM A-2: SYNFUEL BY-PRODUCTS

CHART 1: BENZENE

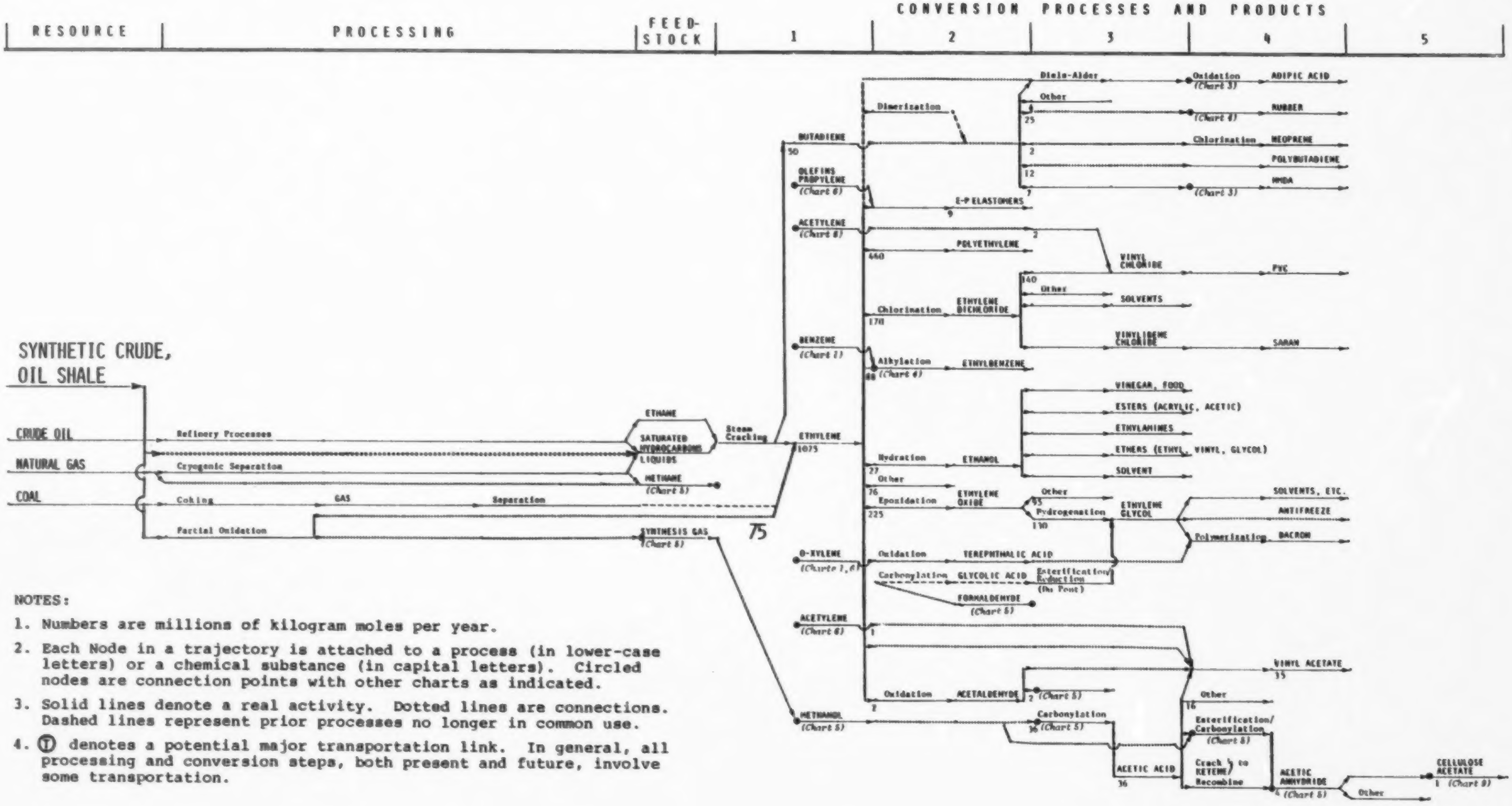

RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL
SHALE, TAR SAND
CRUDE OIL
Partial Oxidation (Chart 5)
Coking
Liquifaction, Hydrocracking
COKE 73%
COKE OVEN GAS 14%
COAL TAR 2%
Distillation
LIGHT OIL 1%
BTX 9/.8/.2
22/2
OTHER
8
4 (Chart 6)
13/2
Refinery Processes
PYROLYSIS GASOLINE
REFORMATE
BTX
APPROXIMATE WT% OF OIL
2%
Separations
90
81
85
2.8%
5%
OTHER FEEDSTOCKS
ENERGY SECTOR
SYNTHESIS GAS (Chart 5)
TOLUENE
84
3 (Chart 6)
Disproportionation
6
29 (Chart 6)
Dealkylation
49
BUTANE
ETHYLENE (Chart 2)
PROPYLENE (Chart 6)
XYLENES
93 (Charts 7,8)
AMMONIA (Chart 5)
BENZENE
137
N-PARAFFINS (Chart 6)
0
3
Oxidation
Oxidation
MALEIC ANHYDRIDE
Alkylation
ETHYLBENZENE (Chart 4)
68
Alkylation
CUMENE
11
8
ISOPROPYL ALCOHOL
26 (Chart 6)
Epoxidation
ACETONE
37
PHENOL
19
Oxidation
ACETIC ACID (Chart 7)
NITROBENZENE
Reduction
13
Hydrogenation
CYCLOHEXANE (Chart 3)
18
Sulfonation
DETERGENTS
Chlorination
CHLOROBENZENE
INSECTICIDES
SOLVENT
Various
33
6.2
8.4
BISPHENOL-A
DIPHENYL CARBONATE
HYDROXY BENZOIC ACID
ANILINE
13
NYLON INTERMEDIATES
4 (Chart 3)
Polymerization
7 (Chart 3)
1
Polymerization
3
EPOXY RESINS
POLYCARBONATE
ASPIRIN
8
URETHANES
DYES
MEDICINE
RUBBER
3

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-2: SYNFUEL BY-PRODUCTS

CHART 2: ETHYLENE

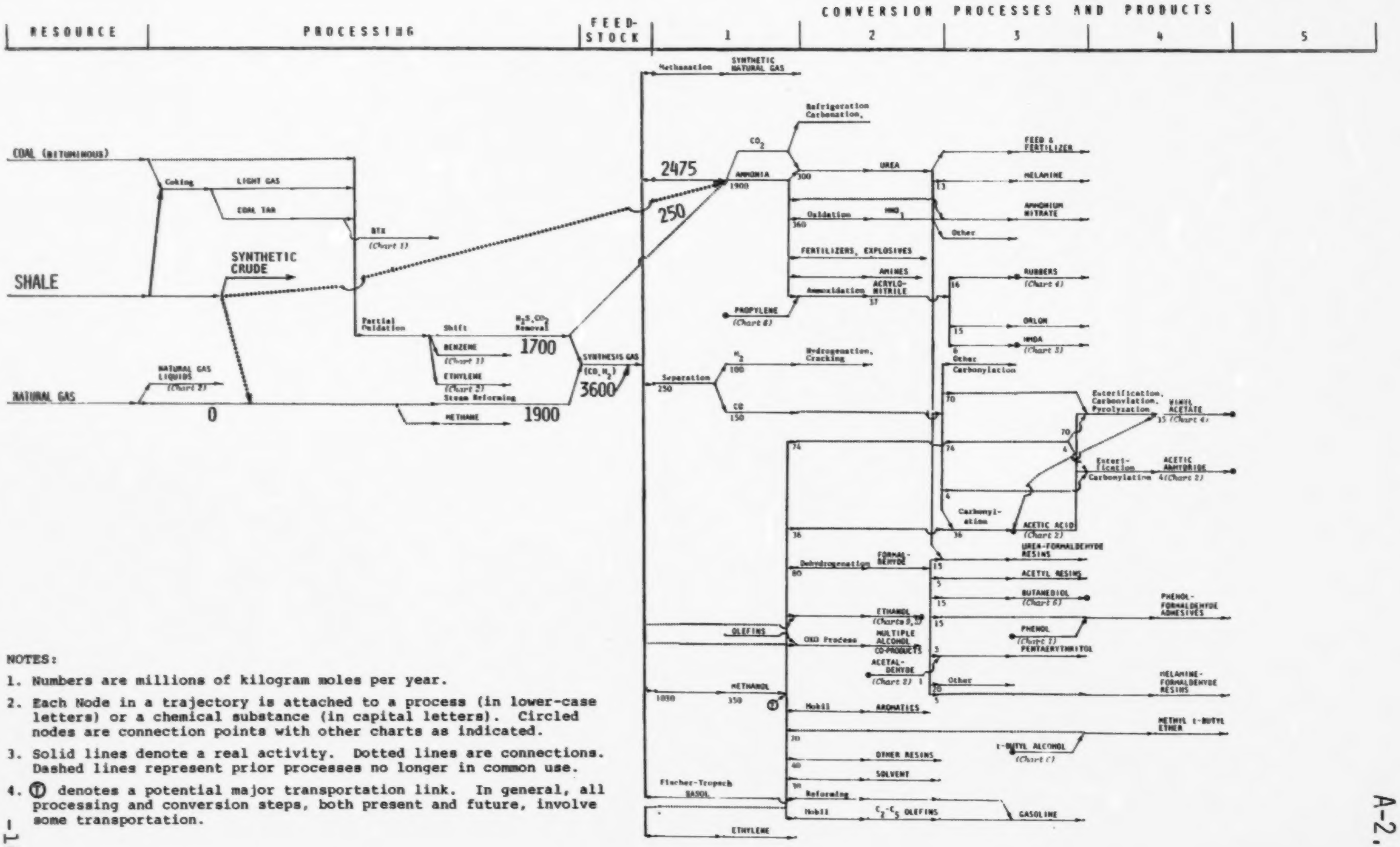

RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
SYNTHETIC CRUDE, OIL SHALE
CRUDE OIL
NATURAL GAS
COAL
Refinery Processes
Cryogenic Separation
Coking
GAS
Separation
Partial Oxidation
ETHANE
SATURATED HYDROCARBONS LIQUIDS
METHANE (Chart 5)
SYNTHESIS GAS (Chart 5)
Steam Cracking
75
BUTADIENE
50
OLEFINS PROPYLENE (Chart 6)
ACETYLENE (Chart 8)
BENZENE (Chart 1)
ETHYLENE
1075
O-XYLENE (Charts 1,6)
ACETYLENE (Chart 8)
METHANOL (Chart 5)
Diels-Alder
Dimerization
Other
4
25
2
12
7
Oxidation (Chart 3)
ADIPIC ACID
(Chart 4)
RUBBER
Chlorination
NEOPRENE
POLYBUTADIENE
(Chart 3)
HMDA
E-P ELASTOMERS
9
2
POLYETHYLENE
440
VINYL CHLORIDE
PVC
140
Other
SOLVENTS
Chlorination
ETHYLENE DICHLORIDE
170
VINYLIDENE CHLORIDE
SARAN
Alkylation (Chart 4)
88
ETHYLBENZENE
VINEGAR, FOOD
ESTERS (ACRYLIC, ACETIC)
ETHYLAMINES
ETHERS (ETHYL, VINYL, GLYCOL)
SOLVENT
Hydration
ETHANOL
27
Other
76
Epoxidation
ETHYLENE OXIDE
225
Other
95
Hydrogenation
130
ETHYLENE GLYCOL
SOLVENTS, ETC.
ANTIFREEZE
Polymerization
DACRON
Oxidation
TEREPHTHALIC ACID
Carbonylation
GLYCOLIC ACID
Esterification/ Reduction (Du Pont)
FORMALDEHYDE (Chart 5)
1
VINYL ACETATE
35
Oxidation
ACETALDEHYDE
2 (Chart 5)
2
Carbonylation
36 (Chart 5)
Other
16
Esterification/ Carbonylation (Chart 8)
ACETIC ACID
36
Crack ½ to KETENE/ Recombine
ACETIC ANHYDRIDE
4 (Chart 5)
Other
CELLULOSE ACETATE
1 (Chart 9)

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-2: SYNFUEL BY-PRODUCTS

CHART 5: SYNTHESIS GAS

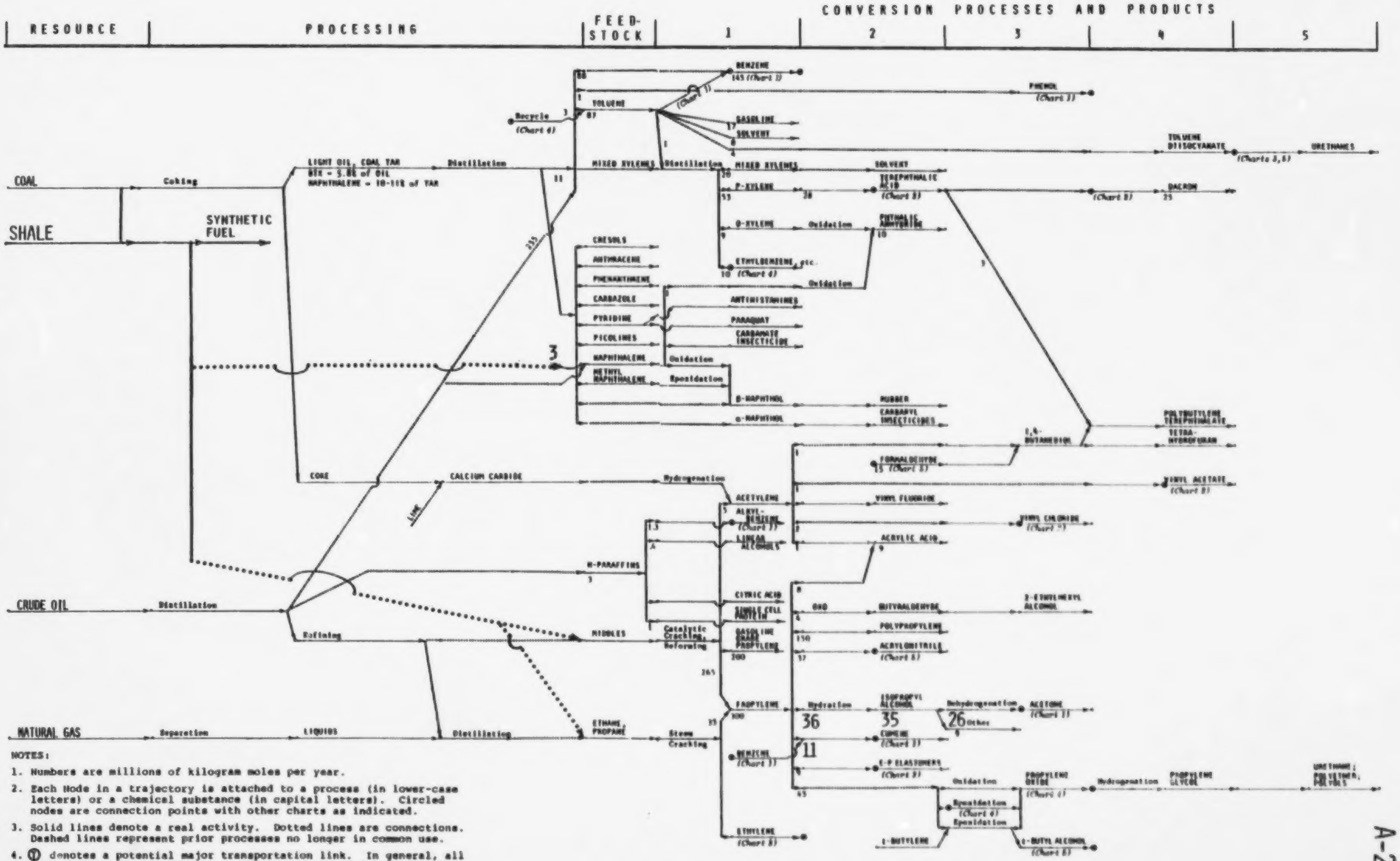

RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL (BITUMINOUS)
SHALE
NATURAL GAS
Coking
LIGHT GAS
COAL TAR
BTX
(Chart 1)
SYNTHETIC CRUDE
NATURAL GAS LIQUIDS
(Chart 2)
0
Partial Oxidation
Shift
H_2S, CO_2 Removal
BENZENE
(Chart 1)
ETHYLENE
(Chart 2)
Steam Reforming
METHANE
1700
1900
SYNTHESIS GAS
(CO, H_2)
3600
2475
250
Methanation
SYNTHETIC NATURAL GAS
Refrigeration Carbonation,
CO_2
AMMONIA
1900
300
UREA
FEED & FERTILIZER
MELAMINE
13
AMMONIUM NITRATE
Oxidation
HNO_3
360
Other
FERTILIZERS, EXPLOSIVES
AMINES
Ammoxidation
ACRYLO-NITRILE
37
PROPYLENE
(Chart 8)
16
RUBBERS
(Chart 4)
15
ORLON
6
HMDA
(Chart 3)
Separation
250
H_2
100
Hydrogenation, Cracking
CO
150
Other
Carbonylation
70
Esterification, Carbonylation, Pyrolyzation
VINYL ACETATE
35 (Chart 4)
70
74
76
4
Esteri-fication
Carbonylation
ACETIC ANHYDRIDE
4 (Chart 2)
4
Carbonyl-ation
ACETIC ACID
(Chart 2)
36
36
Dehydrogenation
FORMAL-DEHYDE
80
15
UREA-FORMALDEHYDE RESINS
5
ACETYL RESINS
15
BUTANEDIOL
(Chart 6)
ETHANOL
(Charts 9, 2)
15
PHENOL-FORMALDEHYDE ADHESIVES
PHENOL
(Chart 1)
OLEFINS
OXO Process
MULTIPLE ALCOHOL CO-PRODUCTS
5
PENTAERYTHRITOL
ACETAL-DEHYDE
(Chart 2)
1
Other
20
5
MELAMINE-FORMALDEHYDE RESINS
METHANOL
1030
350
Ⓣ
Mobil
AROMATICS
METHYL t-BUTYL ETHER
70
t-BUTYL ALCOHOL
(Chart C)
OTHER RESINS
40
SOLVENT
30
Fischer-Tropsch
SASOL
Reforming
Mobil
C_2-C_5 OLEFINS
GASOLINE
ETHYLENE

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-2: SYNFUEL BY-PRODUCTS

CHART 6: OTHER BASIC CHEMICALS

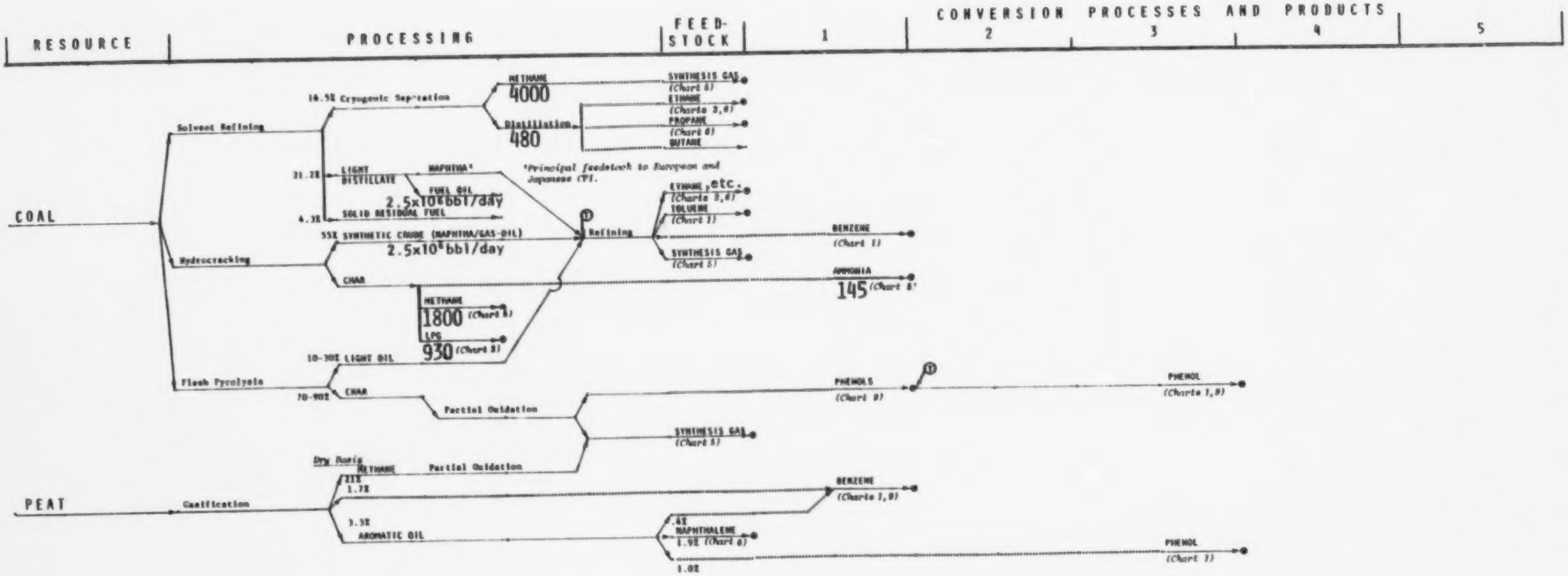

RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL
SHALE
CRUDE OIL
NATURAL GAS
Coking
SYNTHETIC FUEL
LIGHT OIL, COAL TAR
BTX - 5.8% of OIL
NAPHTHALENE - 10-11% of TAR
Distillation
COKE
CALCIUM CARBIDE
LIME
Hydrogenation
Distillation
Refining
Separation
LIQUIDS
Distilling
Recycle
(Chart 4)
BENZENE
145 (Chart 1)
(Chart 1)
PHENOL
(Chart 1)
TOLUENE
87
GASOLINE
SOLVENT
TOLUENE DIISOCYANATE
(Charts 3,5)
URETHANES
MIXED XYLENES
Distillation
MIXED XYLENES
SOLVENT
P-XYLENE
TEREPHTHALIC ACID
(Chart 3)
(Chart 3)
DACRON
25
O-XYLENE
Oxidation
PHTHALIC ANHYDRIDE
ETHYLBENZENE, etc.
(Chart 4)
Oxidation
255
CRESOLS
ANTHRACENE
PHENANTHRENE
CARBAZOLE
PYRIDINE
PICOLINES
NAPHTHALENE
METHYL NAPHTHALENE
ANTIHISTAMINES
PARAQUAT
CARBAMATE INSECTICIDE
Oxidation
Epoxidation
B-NAPHTHOL
α-NAPHTHOL
RUBBER
CARBARYL INSECTICIDES
POLYBUTYLENE TEREPHTHALATE
TETRA-HYDROFURAN
1,4-BUTANEDIOL
FORMALDEHYDE
15 (Chart 3)
VINYL ACETATE
(Chart 3)
ACETYLENE
VINYL FLUORIDE
VINYL CHLORIDE
(Chart 7)
ALKYL-BENZENE
(Chart 7)
LINEAR ALCOHOLS
ACRYLIC ACID
N-PARAFFINS
CITRIC ACID
SINGLE CELL PROTEIN
MIDDLES
Catalytic Cracking, Reforming
GASOLINE SHARE PROPYLENE
200
265
OXO
BUTYRALDEHYDE
2-ETHYLHEXYL ALCOHOL
POLYPROPYLENE
150
ACRYLONITRILE
(Chart 5)
PROPYLENE
300
Hydration
36
ISOPROPYL ALCOHOL
35
Dehydrogenation
ACETONE
(Chart 1)
26 Other
ETHANE, PROPANE
Steam Cracking
CUMENE
(Chart 1)
BENZENE
(Chart 1)
11
E-P ELASTOMERS
(Chart 3)
Oxidation
PROPYLENE OXIDE
(Chart 4)
Hydrogenation
PROPYLENE GLYCOL
URETHANE; POLYETHER, POLYOLS
Epoxidation
(Chart 4)
Epoxidation
ETHYLENE
(Chart 3)
1-BUTYLENE
t-BUTYL ALCOHOL
(Chart 3)
3

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. ① denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-2: SYNFUEL BY-PRODUCTS

CHART 7: COAL, PEAT

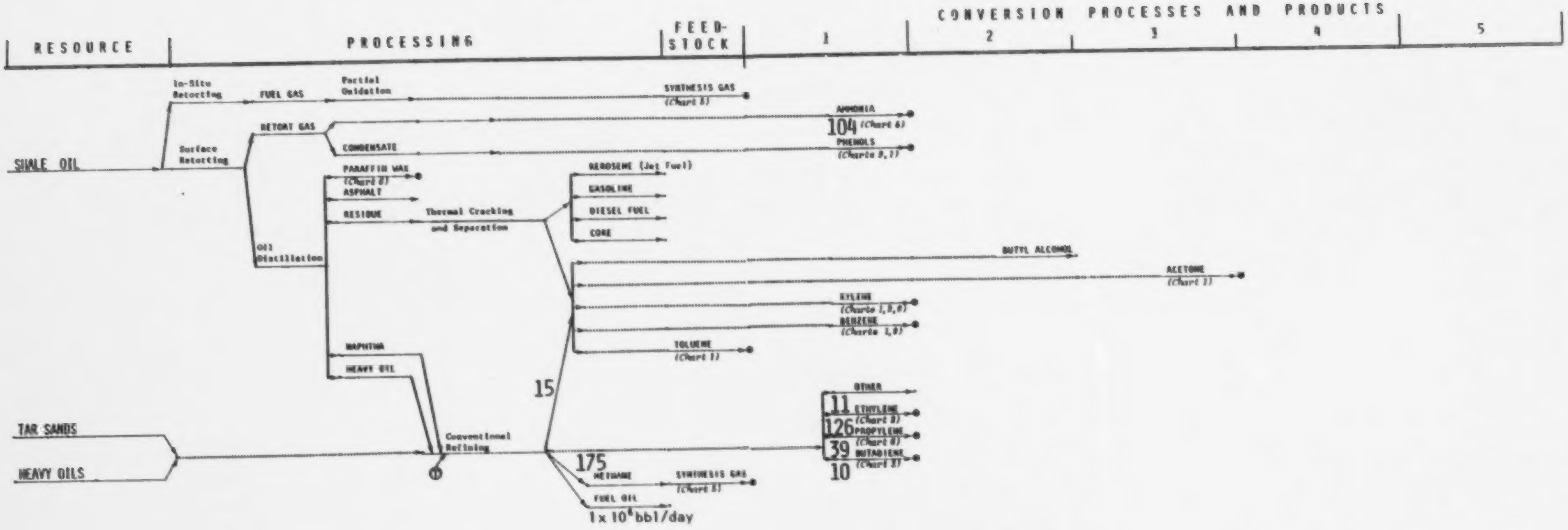

RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL
Solvent Refining
16.5% Cryogenic Separation
METHANE
4000
SYNTHESIS GAS (Chart 5)
Distillation
480
ETHANE (Charts 2,6)
PROPANE (Chart 6)
BUTANE
21.2% LIGHT DISTILLATE
NAPHTHA*
FUEL OIL
2.5x10⁶bbl/day
4.3% SOLID RESIDUAL FUEL
*Principal feedstock to European and Japanese CPI.
Hydrocracking
55% SYNTHETIC CRUDE (NAPHTHA/GAS-OIL)
2.5x10⁶bbl/day
Refining
ETHANE, etc. (Charts 2,6)
TOLUENE (Chart 1)
BENZENE (Chart 1)
SYNTHESIS GAS (Chart 5)
CHAR
AMMONIA
145 (Chart 8)
METHANE
1800 (Chart 6)
LPG
930 (Chart 2)
Flash Pyrolysis
10-30% LIGHT OIL
70-90% CHAR
Partial Oxidation
PHENOLS (Chart 9)
PHENOL (Charts 1,9)
SYNTHESIS GAS (Chart 5)
PEAT
Gasification
Dry Basis
METHANE
21%
Partial Oxidation
1.7%
BENZENE (Charts 1,9)
3.3%
AROMATIC OIL
.4%
NAPHTHALENE
1.9% (Chart 6)
1.0%
PHENOL (Chart 1)

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-2: SYNFUEL BY-PRODUCTS

CHART 8: SHALE OIL, TAR SAND, HEAVY OIL


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
SHALE OIL
In-Situ Retorting
FUEL GAS
Partial Oxidation
SYNTHESIS GAS (Chart 5)
Surface Retorting
RETORT GAS
AMMONIA
104 (Chart 6)
CONDENSATE
PHENOLS (Charts 9, 1)
PARAFFIN WAX (Chart 2)
ASPHALT
RESIDUE
Thermal Cracking and Separation
KEROSENE (Jet Fuel)
GASOLINE
DIESEL FUEL
COKE
Oil Distillation
BUTYL ALCOHOL
ACETONE (Chart 1)
XYLENE (Charts 1,3,8)
BENZENE (Charts 1,8)
TOLUENE (Chart 1)
NAPHTHA
HEAVY OIL
15
TAR SANDS
HEAVY OILS
Conventional Refining
Ⓣ
175
METHANE
SYNTHESIS GAS (Chart 5)
FUEL OIL
1 x 10⁶ bbl/day
OTHER
11
ETHYLENE (Chart 3)
126
PROPYLENE (Chart 8)
39
BUTADIENE (Chart 3)
10

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

C.5. Scenario A-3: Biomass

System A-3 is portrayed in Charts 1, 2, 3, 5, 6, and 9.

The tree has the following prioritized uses:

1. Lignin is processed to meet 100 percent of year 2000 aromatics demand (above the small amount provided from coal tar). Aromatics yield is based on ninety percent recovery of twelve kg moles of aromatic rings per 1955 kg of lignin. Lignin structure is not perfectly known. The rates of the components used in this calculation are based on a portion of a conifer lignin schematic structure (20). Alkylation feeds to create the needed BTX mixture are assumed available from by-products of processing. Additional lignin will be recovered to replace all phenol in 15 million kg mole units of phenol-formaldehyde adhesives (thereby reducing formaldehyde from 28 to eight million kg moles). These uses require 190 billion kg of trees.

2. Hemicellulose associated with this lignin is divided into 15 percent as mannose to cellulose processing and ten percent as xylose.

3. Cellulose is recovered from all trees.

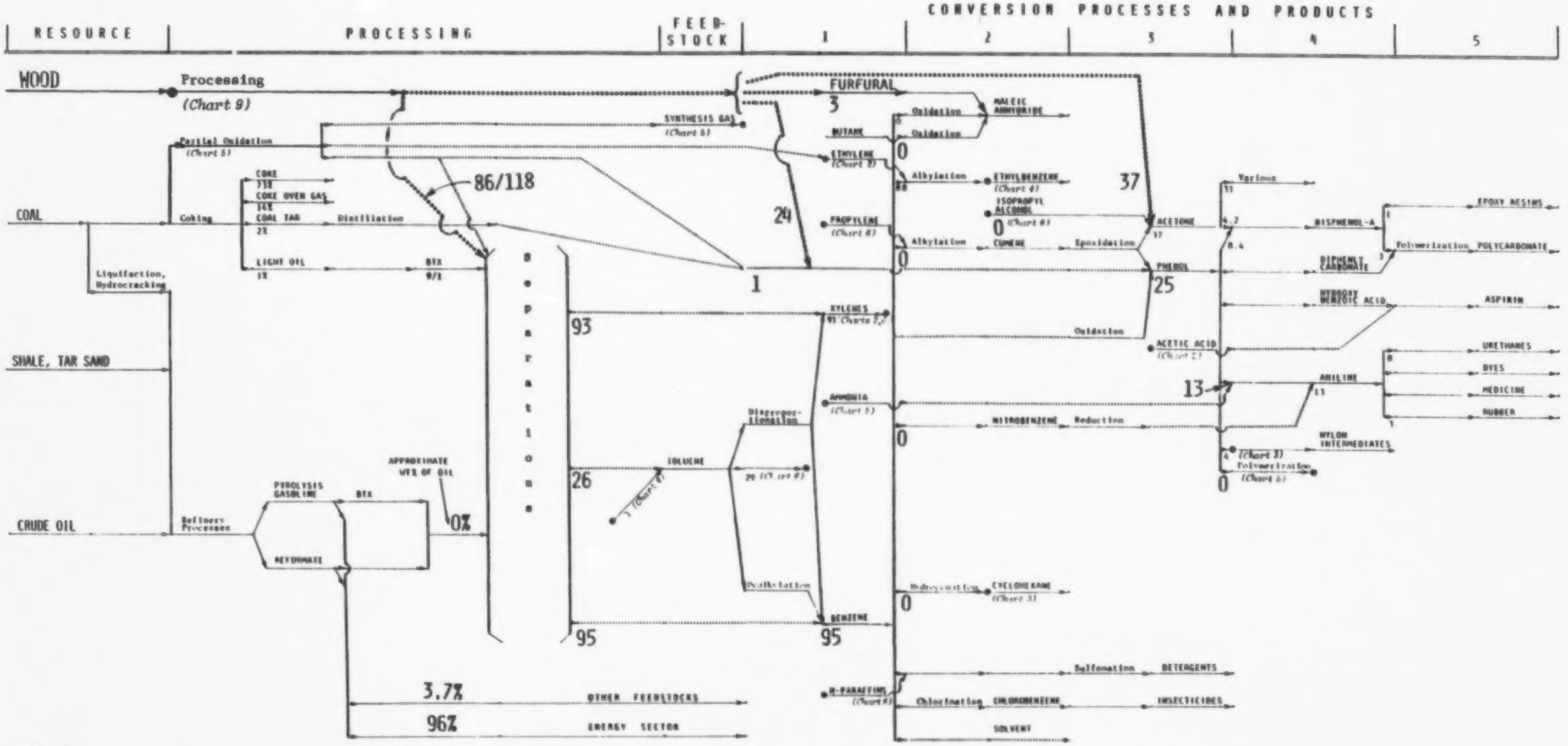
4. The remaining lignin and hemicellulose are pyrolyzed to synthesis gas. (An equivalent assumption would be to process all the hemicellulose but to send a six percent residue from sugar processing to pyrolysis.)

Then the components are subjected to the following chemical reactions:

- Lignin is reacted with formaldehyde to make adhesives;
- Methyl groups are removed from lignin (originally 13 kg mole per 1955 kg), recovered at 95 percent efficiency as methanol;
- Residual lignin is subjected to cleavage by dealkylation or hydrocracking of the C_3 groups (13 kg moles), yielding methane (consumed in subsequent alkylation steps), an ethane/propane mixture used as NGL, and polyhydroxy benzenes (mainly catechol) (originally twelve moles) recovered at 90 percent efficiency. The latter are further processed into phenol, cyclohexane, benzene, toluene and xylenes (saturating all of those markets);
- Cellulose is acid hydrolyzed to levulinic acid (one mole per mole) which may have many uses directly or as 1,4-pentenediol;
- Cellulose is hydrolyzed and fermented to lactic acid (1:1) which may be converted to acrylic acid (saturating the market) and part then to propylene;
- Cellulose is hydrolyzed and fermented to acetone (1:1) (saturating the market);
- Cellulose is hydrolyzed and fermented to ethanol (1:1), with excess beyond the market dehydrated to ethylene. This is a very conservative assumption. The theoretical conversion would be three to one and many studies have been based on between 1.5 and two to one. In addition, the other fermentation processes may make as many moles of ethanol as of the stated products;
- Xylose is acid hydrolyzed to furfural (1:1) which replaces butadiene or is oxidized to maleic acid; and
- Residual lignin and sugars are pyrolyzed to synthesis gas at 47 kg mole per thousand kg sugar and 93 kg mole per thousand kg lignin. There is also an ethylene by-product of 4.6 kg mole per thousand kg lignin.

A very different new future for the supply of aromatics has been collapsed in Chart A-3.1 under the label "processing." The full details are shown on Chart A-3.9. Phenolics from lignin are processed to supply cyclohexane, phenol and aniline directly and then to fill the remaining BTX demands.

SYSTEM A-3: BIOMASS
CHART 1: BENZENE


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
WOOD
Processing
(Chart 9)
COAL
SHALE, TAR SAND
CRUDE OIL
Partial Oxidation
(Chart 5)
Coking
COKE
73%
COKE OVEN GAS
14%
COAL TAR
2%
Distillation
LIGHT OIL
1%
BTX
9/1
Liquifaction, Hydrocracking
86/118
SYNTHESIS GAS
(Chart 5)
FURFURAL
3
Refinery Processes
PYROLYSIS GASOLINE
BTX
REFORMATE
APPROXIMATE WT% OF OIL
0%
Separations
93
26
95
3.7%
OTHER FEEDSTOCKS
96%
ENERGY SECTOR
24
1
BUTANE
ETHYLENE
(Chart 2)
PROPYLENE
(Chart 6)
XYLENES
(Charts 2,6)
TOLUENE
Disproportionation
Dealkylation
29 (Chart 6)
AMMONIA
(Chart 5)
BENZENE
95
N-PARAFFINS
(Chart 6)
Oxidation
Oxidation
MALEIC ANHYDRIDE
0
Alkylation
ETHYLBENZENE
(Chart 4)
ISOPROPYL ALCOHOL
0
(Chart 6)
Alkylation
CUMENE
Epoxidation
0
37
ACETONE
17
PHENOL
25
Oxidation
ACETIC ACID
(Chart 2)
NITROBENZENE
Reduction
0
Hydrogenation
CYCLOHEXANE
(Chart 3)
0
Sulfonation
DETERGENTS
Chlorination
CHLOROBENZENE
INSECTICIDES
SOLVENT
Various
11
4.2
8.4
BISPHENOL-A
DIPHENYL CARBONATE
HYDROXY BENZOIC ACID
13
ANILINE
13
NYLON INTERMEDIATES
4
(Chart 3)
Polymerization
(Chart 6)
0
1
EPOXY RESINS
3
Polymerization
POLYCARBONATE
ASPIRIN
8
URETHANES
DYES
MEDICINE
RUBBER
1

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

Phenol's former coproduct, acetone, is now fully supplied from cellulose fermentation.

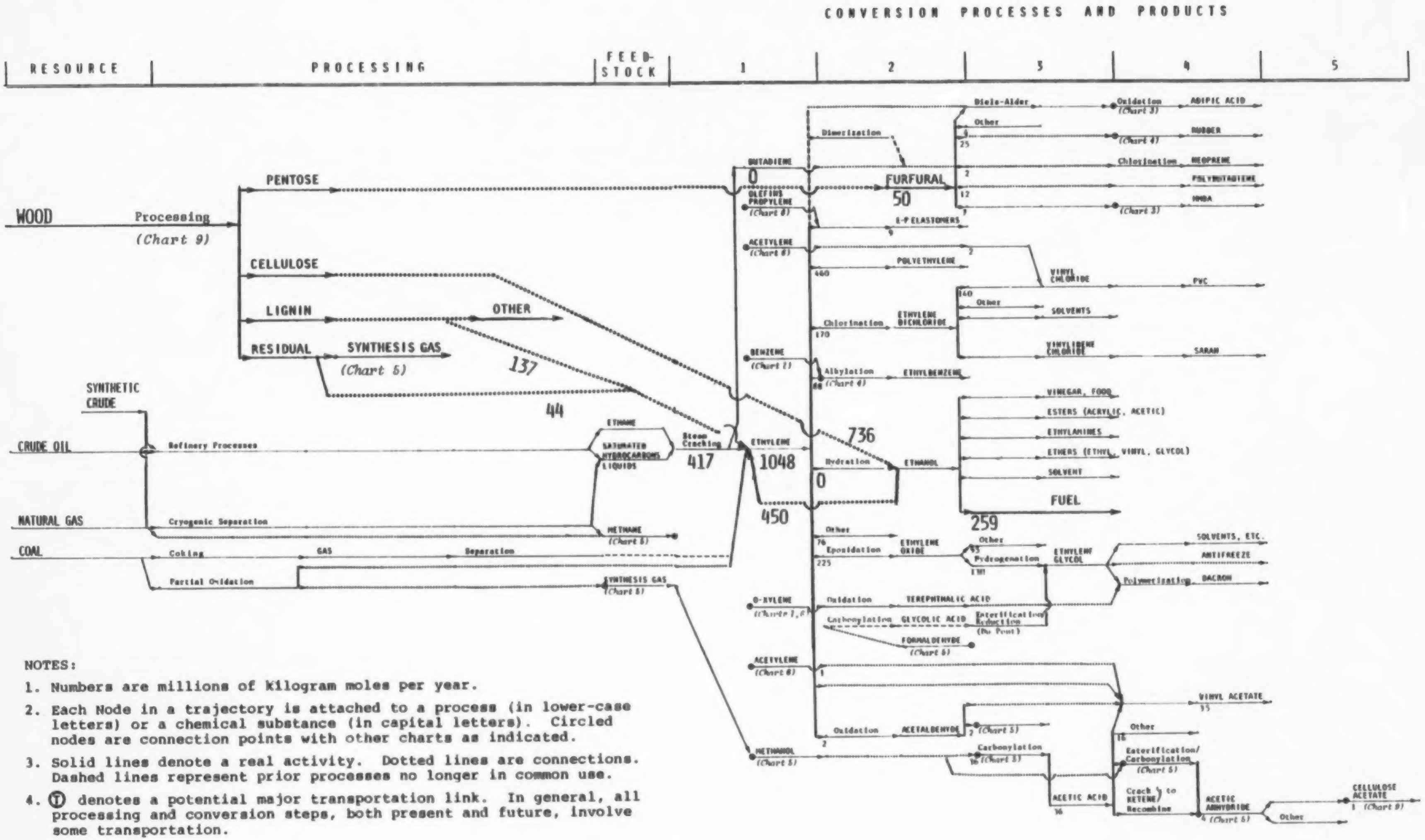
In Chart A-3.2, ethanol from cellulose supplies a large part of the gasohol market as well as the chemical and food markets. But still over sixty percent remains and is catalytically dehydrated to ethylene. Processing of lignin and partial oxidation of the residues also provide ethane and ethylene, so the ethylene which must be derived from traditional sources is greatly reduced.

Chart A-3.3 shows that two major varieties of polyamide (nylons) can be totally wood based. Chart A-3.5 shows an altered methanol system, with a decline in the formaldehyde market, a major non-synthesis gas methanol supply, and wholly new sources supplying that syngas which is needed. As mentioned above, ammonia would hold on to methane-based syngas because of the more favorable H_2/CO ratio. Chart A-3.6 reiterates the changes involving propylene and aromatics. Note that in providing ethanol, lactic acid and furfural, wood substitutes a new two to four carbon family for the traditional ethylene/propylene/butadiene family from catalytic crackers.

Chart A-3.9 shows the myriad chemical products possible from tree processing. Many of the chemicals appear at levels which conflict with the present chemical system; connecting arrows are shown with reversed directions. Chart A-3.9 also shows several additional conversion processes, which have not been discussed here, and their potential chemical products.

SYSTEM A-3: BIOMASS

CHART 2: ETHYLENE


CONVERSION PROCESSES AND PRODUCTS
RESOURCE
PROCESSING
FEED-STOCK
1
2
3
4
5
WOOD
Processing
(Chart 9)
PENTOSE
CELLULOSE
LIGNIN
OTHER
RESIDUAL
SYNTHESIS GAS
(Chart 5)
137
44
SYNTHETIC CRUDE
CRUDE OIL
Refinery Processes
ETHANE
SATURATED HYDROCARBONS
LIQUIDS
Steam Cracking
417
NATURAL GAS
Cryogenic Separation
METHANE
(Chart 5)
COAL
Coking
GAS
Separation
Partial Oxidation
SYNTHESIS GAS
(Chart 5)
BUTADIENE
0
OLEFINS PROPYLENE
(Chart 8)
ACETYLENE
(Chart 8)
BENZENE
(Chart 1)
ETHYLENE
1048
450
O-XYLENE
(Charts 1,6)
ACETYLENE
(Chart 8)
METHANOL
(Chart 5)
Diels-Alder
Dimerization
Other
FURFURAL
50
E-P ELASTOMERS
POLYETHYLENE
460
Chlorination
170
ETHYLENE DICHLORIDE
Alkylation
(Chart 4)
ETHYLBENZENE
736
Hydration
0
ETHANOL
Other
76
Epoxidation
225
ETHYLENE OXIDE
Oxidation
TEREPHTHALIC ACID
Carbonylation
GLYCOLIC ACID
Esterification Reduction
(Du Pont)
FORMALDEHYDE
(Chart 5)
1
Oxidation
2
ACETALDEHYDE
2
(Chart 5)
Carbonylation
(Chart 5)
25
2
12
7
9
2
VINYL CHLORIDE
140
Other
SOLVENTS
VINYLIDENE CHLORIDE
VINEGAR, FOOD
ESTERS (ACRYLIC, ACETIC)
ETHYLAMINES
ETHERS (ETHYL, VINYL, GLYCOL)
SOLVENT
FUEL
259
Other
Hydrogenation
ETHYLENE GLYCOL
ACETIC ACID
16
Other
16
Esterification/ Carbonylation
(Chart 5)
Crack to KETENE Recombine
ACETIC ANHYDRIDE
4 (Chart 5)
Other
Oxidation
(Chart 3)
ADIPIC ACID
(Chart 4)
RUBBER
Chlorination
NEOPRENE
POLYBUTADIENE
(Chart 3)
HMDA
PVC
SARAN
SOLVENTS, ETC.
ANTIFREEZE
Polymerization
DACRON
VINYL ACETATE
35
CELLULOSE ACETATE
1 (Chart 9)

NOTES:

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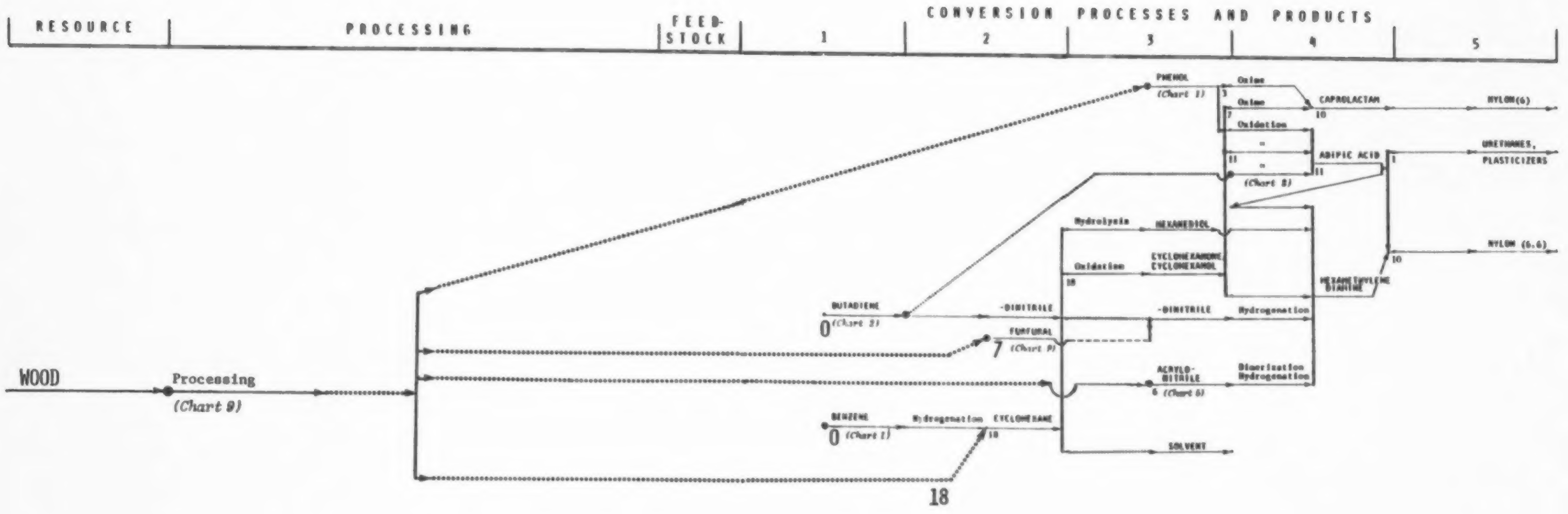
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-3: BIOMASS

CHART 3: CYCLOHEXANE

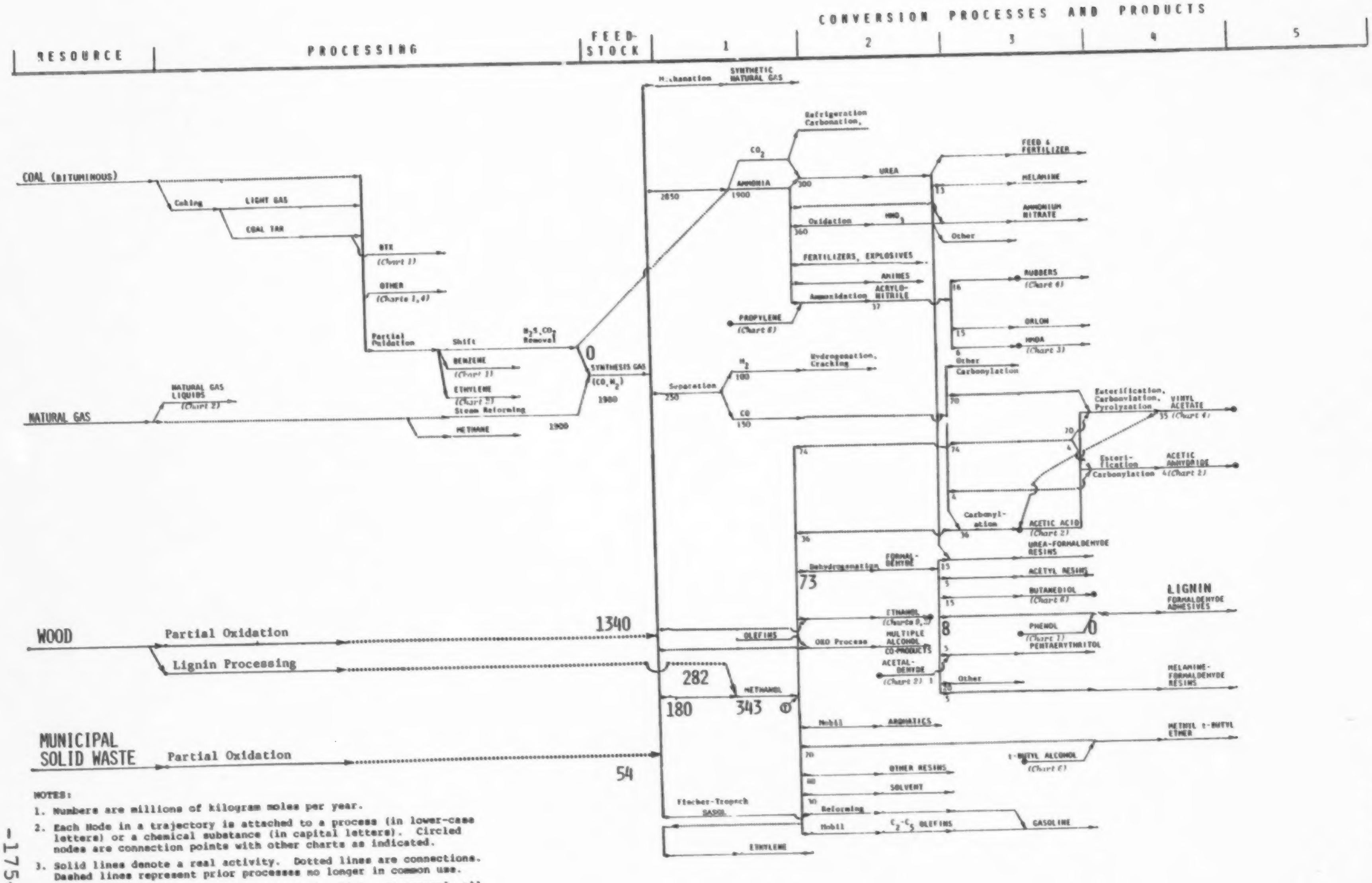

RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
WOOD
Processing
(Chart 9)
PHENOL
(Chart 1)
Oxime
Oxime
3
7
CAPROLACTAM
10
NYLON(6)
Oxidation
"
"
11
11
ADIPIC ACID
(Chart 8)
1
URETHANES,
PLASTICIZERS
NYLON (6,6)
10
Hydrolysis
HEXANEDIOL
Oxidation
CYCLOHEXANONE/
CYCLOHEXANOL
18
HEXAMETHYLENE
DIAMINE
BUTADIENE
0 (Chart 2)
-DINITRILE
-DINITRILE
Hydrogenation
FURFURAL
7 (Chart 9)
ACRYLO-
NITRILE
6 (Chart 6)
Dimerization
Hydrogenation
BENZENE
0 (Chart 1)
Hydrogenation
CYCLOHEXANE
18
SOLVENT
18

NOTES:

1. Numbers are millions of kilogram moles per year.
2. Each Node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as indicated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-3: BIOMASS

CHART 5: SYNTHESIS GAS


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL (BITUMINOUS)
Coking
LIGHT GAS
COAL TAR
BTX
(Chart 1)
OTHER
(Charts 1,4)
Partial Oxidation
Shift
H_2S, CO_2 Removal
BENZENE
(Chart 1)
ETHYLENE
(Chart 2)
Steam Reforming
NATURAL GAS
NATURAL GAS LIQUIDS
(Chart 2)
METHANE
1900
0
SYNTHESIS GAS
(CO, H_2)
1900
Methanation
SYNTHETIC NATURAL GAS
2850
AMMONIA
1900
CO_2
Refrigeration Carbonation,
300
UREA
FEED & FERTILIZER
MELAMINE
13
AMMONIUM NITRATE
Other
Oxidation
HNO_3
360
FERTILIZERS, EXPLOSIVES
AMINES
Ammoxidation
ACRYLO-NITRILE
37
PROPYLENE
(Chart 6)
16
RUBBERS
(Chart 6)
15
ORLON
6
HMDA
(Chart 3)
Separation
250
H_2
100
Hydrogenation, Cracking
CO
150
Other Carbonylation
70
Esterification, Carbonylation, Pyrolyzation
VINYL ACETATE
35 (Chart 4)
70
74
74
4
Esteri-fication
Carbonylation
ACETIC ANHYDRIDE
4 (Chart 2)
4
Carbonyl-ation
ACETIC ACID
(Chart 2)
36
36
UREA-FORMALDEHYDE RESINS
Dehydrogenation
FORMAL-DEHYDE
73
15
ACETYL RESINS
5
BUTANEDIOL
(Chart 6)
15
LIGNIN
FORMALDEHYDE ADHESIVES
ETHANOL
(Charts 8, 2)
8
PHENOL
(Chart 1)
0
OLEFINS
OXO Process
MULTIPLE ALCOHOL CO-PRODUCTS
5
PENTAERYTHRITOL
ACETAL-DEHYDE
(Chart 2) 1
Other
20
5
MELAMINE-FORMALDEHYDE RESINS
WOOD
Partial Oxidation
Lignin Processing
1340
282
METHANOL
180
343
Ⓣ
Mobil
AROMATICS
METHYL t-BUTYL ETHER
70
t-BUTYL ALCOHOL
(Chart 6)
OTHER RESINS
40
SOLVENT
30
Reforming
Mobil
C_2-C_5 OLEFINS
GASOLINE
MUNICIPAL SOLID WASTE
Partial Oxidation
54
Fischer-Tropsch SASOL
ETHYLENE

NOTES:

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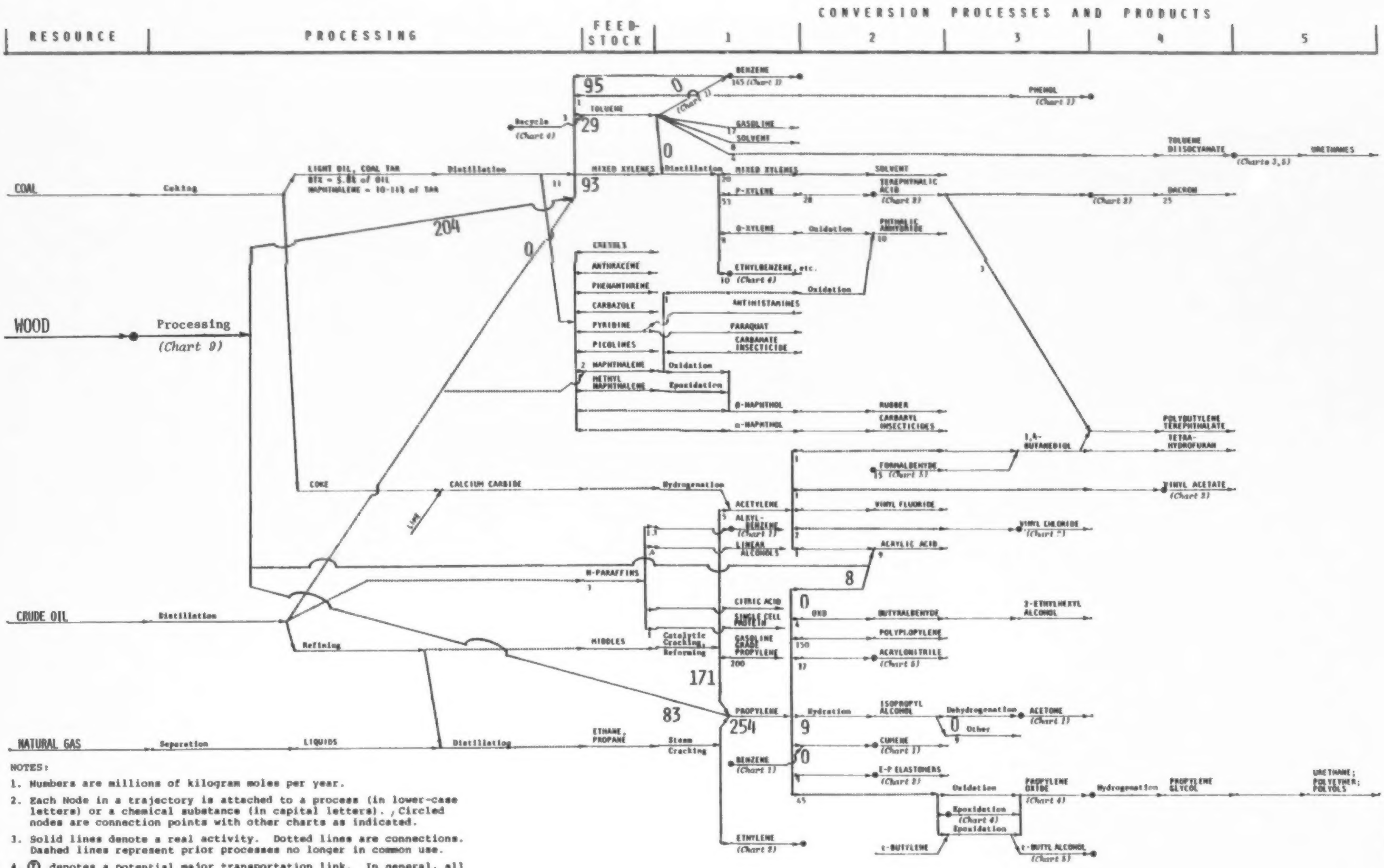
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-3: BIOMASS

CHART 6: OTHER BASIC CHEMICALS


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
COAL
Coking
LIGHT OIL, COAL TAR
BTX = 5.8% of OIL
NAPHTHALENE = 10-11% of TAR
Distillation
WOOD
Processing
(Chart 9)
CRUDE OIL
Distillation
Refining
NATURAL GAS
Separation
LIQUIDS
Distillating
95
29
93
204
0
11
Recycle
(Chart 4)
TOLUENE
MIXED XYLENES
Distillation
BENZENE
145 (Chart 1)
(Chart 1)
PHENOL
(Chart 1)
GASOLINE
17
SOLVENT
8
4
TOLUENE DIISOCYANATE
(Charts 3,5)
URETHANES
MIXED XYLENES
20
SOLVENT
P-XYLENE
53
28
TEREPHTHALIC ACID
(Chart 2)
(Chart 2)
DACRON
25
O-XYLENE
9
Oxidation
PHTHALIC ANHYDRIDE
10
ETHYLBENZENE, etc.
10 (Chart 4)
Oxidation
3
CRESOLS
ANTHRACENE
PHENANTHRENE
CARBAZOLE
PYRIDINE
PICOLINES
2 NAPHTHALENE
METHYL NAPHTHALENE
ANTIHISTAMINES
PARAQUAT
CARBAMATE INSECTICIDE
Oxidation
Epoxidation
β-NAPHTHOL
α-NAPHTHOL
RUBBER
CARBARYL INSECTICIDES
POLYBUTYLENE TEREPHTHALATE
TETRA-HYDROFURAN
1,4-BUTANEDIOL
FORMALDEHYDE
15 (Chart 5)
VINYL ACETATE
(Chart 2)
COKE
CALCIUM CARBIDE
LIME
Hydrogenation
ACETYLENE
5 ALKYL-BENZENE
(Chart 1)
LINEAR ALCOHOLS
13
4
N-PARAFFINS
3
VINYL FLUORIDE
VINYL CHLORIDE
(Chart 7)
ACRYLIC ACID
9
8
CITRIC ACID
SINGLE CELL PROTEIN
GASOLINE GRADE PROPYLENE
200
MIDDLES
Catalytic Cracking,
Reforming
171
83
0
OXO
4
BUTYRALDEHYDE
2-ETHYLHEXYL ALCOHOL
POLYPROPYLENE
150
ACRYLONITRILE
(Chart 5)
37
ETHANE, PROPANE
Steam Cracking
PROPYLENE
254
Hydration
9
ISOPROPYL ALCOHOL
Dehydrogenation
0
Other
9
ACETONE
(Chart 1)
CUMENE
(Chart 1)
BENZENE
(Chart 1)
0
E-P ELASTOMERS
(Chart 2)
45
Oxidation
PROPYLENE OXIDE
(Chart 4)
Hydrogenation
PROPYLENE GLYCOL
URETHANE; POLYETHER; POLYOLS
Epoxidation
(Chart 4)
Epoxidation
t-BUTYLENE
t-BUTYL ALCOHOL
(Chart 5)
ETHYLENE
(Chart 2)

NOTES:

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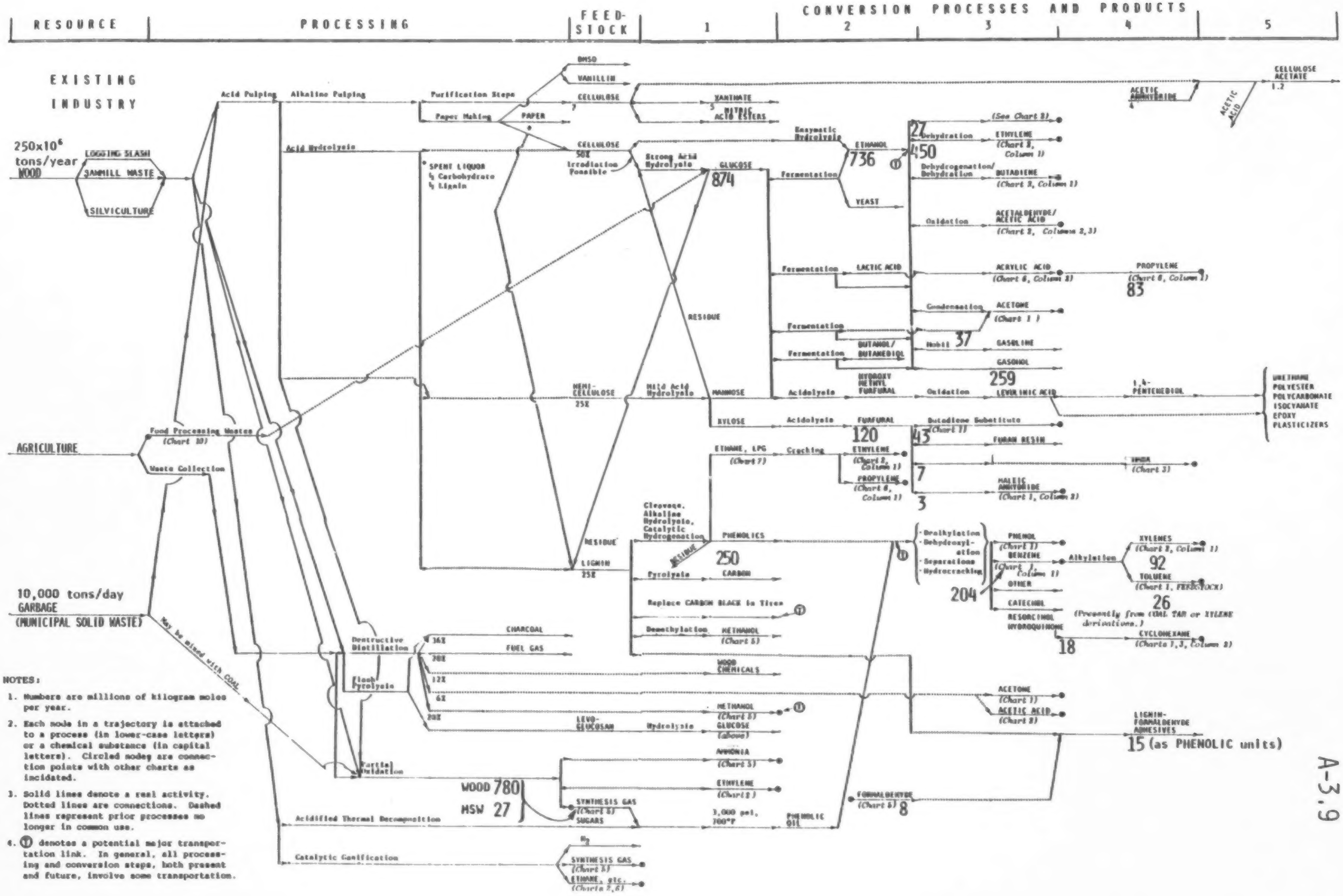
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

SYSTEM A-3: BIOMASS

CHART 9: WOOD, DRY BIOMASS


RESOURCE
PROCESSING
FEED-STOCK
CONVERSION PROCESSES AND PRODUCTS
1
2
3
4
5
EXISTING INDUSTRY
250x10⁶ tons/year WOOD
LOGGING SLASH
SAWMILL WASTE
SILVICULTURE
AGRICULTURE
Food Processing Wastes (Chart 10)
Waste Collection
10,000 tons/day GARBAGE (MUNICIPAL SOLID WASTE)
May be mixed with COAL
Acid Pulping
Alkaline Pulping
Acid Hydrolysis
Purification Steps
Paper Making
PAPER
SPENT LIQUOR ½ Carbohydrate ½ Lignin
DMSO
VANILLIN
CELLULOSE
CELLULOSE 50%
Irradiation Possible
HEMI-CELLULOSE 25%
RESIDUE
LIGNIN 25%
XANTHATE
NITRIC ACID ESTERS
Enzymatic Hydrolysis
Strong Acid Hydrolysis
GLUCOSE
874
Mild Acid Hydrolysis
MANNOSE
XYLOSE
RESIDUE
Fermentation
ETHANOL
736
YEAST
27
450
(See Chart 2)
Dehydration
ETHYLENE (Chart 2, Column 1)
Dehydrogenation/Dehydration
BUTADIENE (Chart 2, Column 1)
Oxidation
ACETALDEHYDE/ACETIC ACID (Chart 2, Columns 2,3)
Fermentation
LACTIC ACID
ACRYLIC ACID (Chart 6, Column 2)
PROPYLENE (Chart 6, Column 1)
83
Condensation
ACETONE (Chart 1)
Fermentation
BUTANOL/BUTANEDIOL
Fermentation
Mobil
37
GASOLINE
GASOHOL
259
Acidolysis
HYDROXY METHYL FURFURAL
Oxidation
LEVULINIC ACID
1,4-PENTENEDIOL
URETHANE
POLYESTER
POLYCARBONATE
ISOCYANATE
EPOXY
PLASTICIZERS
Acidolysis
FURFURAL
120
43
Butadiene Substitute (Chart 1)
FURAN RESIN
7
HMDA (Chart 3)
3
MALEIC ANHYDRIDE (Chart 1, Column 2)
ETHANE, LPG (Chart 7)
Cracking
ETHYLENE (Chart 2, Column 1)
PROPYLENE (Chart 6, Column 1)
ACETIC ANHYDRIDE
4
ACETIC ACID
CELLULOSE ACETATE
1.2
Cleavage, Alkaline Hydrolysis, Catalytic Hydrogenation
PHENOLICS
250
RESIDUE
Pyrolysis
CARBON
Replace CARBON BLACK in Tires
Demethylation
METHANOL (Chart 5)
Dealkylation
Dehydroxylation
Separations
Hydrocracking
PHENOL (Chart 1)
BENZENE (Chart 1, Column 1)
OTHER
CATECHOL
RESORCINOL
HYDROQUINONE
204
Alkylation
XYLENES (Chart 2, Column 1)
92
TOLUENE (Chart 1, FEEDSTOCK)
26
(Presently from COAL TAR or XYLENE derivatives.)
CYCLOHEXANE (Charts 1,3, Column 2)
18
Destructive Distillation
Flash Pyrolysis
36%
20%
12%
6%
20%
CHARCOAL
FUEL GAS
WOOD CHEMICALS
METHANOL (Chart 5)
LEVO-GLUCOSAN
Hydrolysis
GLUCOSE (above)
ACETONE (Chart 1)
ACETIC ACID (Chart 2)
LIGNIN-FORMALDEHYDE ADHESIVES
15 (as PHENOLIC units)
Partial Oxidation
WOOD 780
MSW 27
AMMONIA (Chart 5)
ETHYLENE (Chart 2)
SYNTHESIS GAS (Chart 5)
SUGARS
Acidified Thermal Decomposition
3,000 psi, 700°F
PHENOLIC OIL
FORMALDEHYDE (Chart 5)
8
Catalytic Gasification
H₂
SYNTHESIS GAS (Chart 5)
ETHANE, etc. (Charts 2,6)
Ⓣ

NOTES:

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2. Each node in a trajectory is attached to a process (in lower-case letters) or a chemical substance (in capital letters). Circled nodes are connection points with other charts as incidated.
3. Solid lines denote a real activity. Dotted lines are connections. Dashed lines represent prior processes no longer in common use.
4. Ⓣ denotes a potential major transportation link. In general, all processing and conversion steps, both present and future, involve some transportation.

Those processes are less likely to be important as feedstock sources, but, nevertheless, no important environmental consequences are foreseen. Not shown is the possibility of obtaining oil-like substances directly from plants, i.e., as a plant secretion rather than a transformation of the plant structure. Among the plants under study are guayule, jojoba, yucca, euphorbia, and milkweed. Neither the timing nor the probable scale of their eventual use warrants more than cursory monitoring of research progress.

Further, System R-1980 has Chart 10 (see Section C.1) which shows additional biomass sources and conversion processes appropriate for very wet materials. The anerobic digestion of manure is now commonly used in other countries and increasingly in the United States to supply rural fuel needs. Simplex/Sylplex (briquettes made from coal and sewage sludge, mixed with air-classified garbage or shredded wood, and pyrolyzed in a slagging gasifier) has been proposed as a generator of gas for electric power plants. However, various problems -- such as product purity, scale, low pressure and managing large scale aquaculture -- put these sources of feedstocks well into the next century.

REFERENCES

(1) Chemical Marketing Reporter. Jan. 19, 1981. p. 7.

(2) Sherwin, M.B., and M.E. Frank. Chemicals From Oil and Shale - an R&D Analysis for National Science Foundation. Chem Systems Inc., New York. June 1975.

(3) Mills, J. Foam Insulation Industry Says It's Reeling. Washington Post. March 28, 1981.

APPENDIX D. TECHNOLOGIES FOR ALTERNATIVE FUTURES

At this time, the research emphasis in the government, academic and business communities is on identifying and developing technically feasible processes for turning non-oil-and-gas hydrocarbons into chemical feedstocks. Major studies have been and will continue to be made to survey these technologies, estimate their economics and assess their future impacts (1,2,3). Implementation of these technologies is, for the most part, still years away.

This report concludes that many of the new feedstocks will be by-products of the energy industry, closely resembling current feedstocks, and will be processed conventionally. Thus, in order to identify possible new environmental hazards, the emphasis has been on processes which convert an alternative source material primarily to chemicals.

Following are descriptive details on several of the processes discussed in the main text.

D.1. Methanol Based Chemical Plant

Methanol conversions into industrial chemicals are taking on new importance as petroleum prices continue to rise and catalyst technology improves.

Methanol is manufactured through a shift reaction from gas derived from the controlled combustion of coal (pyrolysis). This gas (known as synthesis gas) may alternatively be used in a Fischer-Tropsch process for direct conversion into a broad spectrum of olefins from LPG to waxy oils. The nature of the Fischer-Tropsch catalyst precludes any further selectivity or specificity in the nature of compound created. A typical, commercial-scaled Fischer-Tropsch plant is the South African Synthetic Gas and Oil Company's Sasol I complex, which was designed to produce fuels. A typical output stream of Sasol I is as follows:

	SASOL I	MOBIL
	(weight percent)	
Light Gas C_1-C_2	20.1	1.3
LPG C_3-C_4	23.0	17.8
Gasoline C_5-C_{12}	39.0	80.9
Diesel C_{13}-C_{18}	5.0	0
Heavy Oil C_{19}+	6.0	0
O-Compounds	7.0	0
Aromatics, % of gasoline	5	38.6

The low degree of selectivity of Fischer-Tropsch can be seen through the isolation of the heavier petroleum fractions.

By contrast, a process developed by Mobil exhibits a high degree of selectivity, yielding 80.9 percent gasoline with 38.6 percent aromatic composition. This process uses a shape selective zeolite catalyst with methanol as the feedstock.

The absence of the heavier oils from the product stream makes the process attractive to industry. Lighter portions are easily marketable or reformed into other chemicals.

The conversion of coal to methanol begins with pyrolysis. A number of different types of gasifiers have been studied. The synthesis gas is then fed to a sulfur recovery unit where the bulk of the sulfur is removed. Residual sulfur is removed over zinc oxide. Complete sulfur removal is required, as the shift conversion catalysts are sensitive to sulfur poisoning.

After separation, the carbon monoxide and hydrogen mixture is fed through a fluidized catalyst bed and then methanol is condensed from the effluent gases. Large research efforts are being devoted to the development of new catalysts. This work must be monitored closely as changes in catalysts can affect the chemical forms produced in the process, with attendant environmental risk, and can lead to other environmental problems associated with catalyst regeneration or disposal.

After synthesis, methanol can be fed to reactions resulting in the production of ethanol, ethylene, acetic acid, ethylene glycol, or gasoline (Mobil). The gasoline fraction, which is 38.6 percent aromatic, can be further separated, with toluene going to styrene synthesis. The lighter fractions can be subjected to cracking and reforming, or used directly as fuel.

D.2. Wood Chemicals

The principle chemical produced from ethanol is ethylene by dehydration. Prior to 1945 a significant portion (although not large compared to present production) of the world's production of ethylene was produced by this reaction of ethanol. Later the large scale thermal cracking of cheap hydrocarbons made this process uneconomical. With the advent of new catalysts that have a greater resistance to fouling and an ethylene selectivity of about 97 percent, ethanol dehydration is becoming competitive with petroleum cracking as a source of ethylene (5). Even the reactor size and subsequent capital investment needed for ethylene production have been decreased by the greater efficiency of the catalyst. The resultant product ethylene is about 99.8 mole percent pure with ethane as the major contaminant. Minor process design changes will upgrade the product to the 99.95 percent purity required for polyethylene manufacture.

A modern plant dehydrating ethanol to ethylene will require 1.73 kg ethanol per kilogram of ethylene produced, with catalyst and chemicals costing five dollars.

Conversion of lignin into chemicals such as phenols, benzene and related aromatics is not well characterized and potential waste streams are not identified. The void is primarily due to a definite lack of research into industrial conversion methods that would be used to produce these products. Theoretical processes have been outlined by Goldstein, Pearl and numerous Russian scientists with no mention of waste streams associated with each step of the process. It is suspected that no insurmountable or untreatable waste stream would be created by lignin processing. Conversion reactions use hydrogenation, hydrolysis, dehydrogenation, dealkylation and hydrocracking. Waste streams are thus not expected to differ in character from those in the petrochemical industry.

Research into new fermentation technology shows promise in directing pentosans into chemicals other than furfural. Research completed by Wang, et al., at MIT in 1978 indicates certain thermophilic bacteria can ferment xylose and other pentosans into acetic acid, butanol, acetone, lactic acid, acrylic acid and ethanol. Optimism is expressed that quantity production technology will be available in the near future.

Problems with these fermentation reactions are associated with organism tolerance to their metabolic by-products that are the fruits of their cultivation. Variation of the incubation temperature has been useful in delaying toxic reactions to product. New strains of product tolerant bacteria are also on the horizon. An acetate tolerant strain of Clostridium Thermoacetium has been isolated. This bacteria will tolerate acetate concentrations of up to 60 kilogram/cubic meter before total growth inhibition results. Artificial selection and genetic engineering are likely to be instrumental in a breakthrough in this area.

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5. Kochar, N.K., and R.L. Marcell. Ethylene from Ethanol: The Economics are Improved. Chemical Engineering, January 28, 1980. pp. 80-81.

APPENDIX E. ENVIRONMENTAL COEFFICIENTS

Figures E.1, E.2, and E.3 summarize all process trajectories leading to the five key chemicals. As will be discussed below on a case-by-case basis, not all trajectories are relevant for all scenarios. As feedstocks change, the processes and trajectories used change as well. Also not all trajectories are of equal environmental importance. Some contain processes that are environmentally benign, while others are potentially quite harmful.

In accordance with the RMS format, each trajectory is examined for residuals of environmental concern. The residuals are expressed in units of residual per unit of product derived. Coefficients derived in this manner can be used to obtain a residual stream peculiar to the production of any or all of the five target chemicals.

E.1. R-1980

As explained in Section 1.2.1, R-1980 portrays the baseline chemical system -- industry flows as they currently exist. The sections below examine the environmental coefficients for the scenario on a chemical-by-chemical basis.

(a) Benzene. Today approximately 93 percent of all benzene is manufactured starting from petroleum, the remaining seven

Figure E.1. Collected Benzene Trajectories

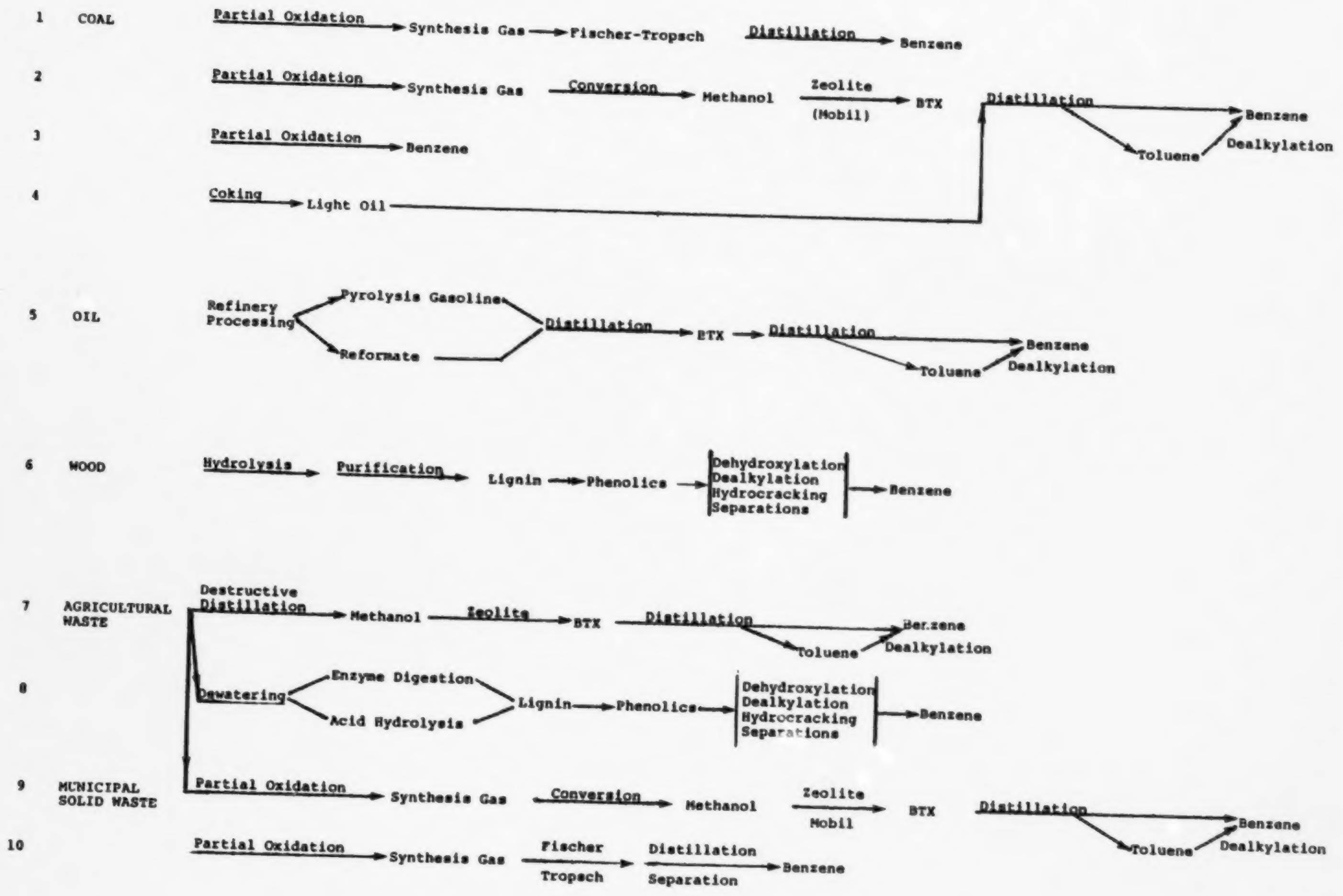

1 COAL
Partial Oxidation
Synthesis Gas
Fischer-Tropsch
Distillation
Benzene
2
Partial Oxidation
Synthesis Gas
Conversion
Methanol
Zeolite
(Mobil)
BTX
Distillation
Benzene
Toluene
Dealkylation
3
Partial Oxidation
Benzene
4
Coking
Light Oil
5 OIL
Refinery Processing
Pyrolysis Gasoline
Reformate
Distillation
BTX
Distillation
Benzene
Toluene
Dealkylation
6 WOOD
Hydrolysis
Purification
Lignin
Phenolics
Dehydroxylation
Dealkylation
Hydrocracking
Separations
Benzene
7 AGRICULTURAL WASTE
Destructive Distillation
Methanol
Zeolite
BTX
Distillation
Benzene
Toluene
Dealkylation
8
Dewatering
Enzyme Digestion
Acid Hydrolysis
Lignin
Phenolics
Dehydroxylation
Dealkylation
Hydrocracking
Separations
Benzene
9 MUNICIPAL SOLID WASTE
Partial Oxidation
Synthesis Gas
Conversion
Methanol
Zeolite
Mobil
BTX
Distillation
Benzene
Toluene
Dealkylation
10
Partial Oxidation
Synthesis Gas
Fischer
Tropsch
Distillation
Separation
Benzene

Figure E.2. Collected Ethylene Trajectories

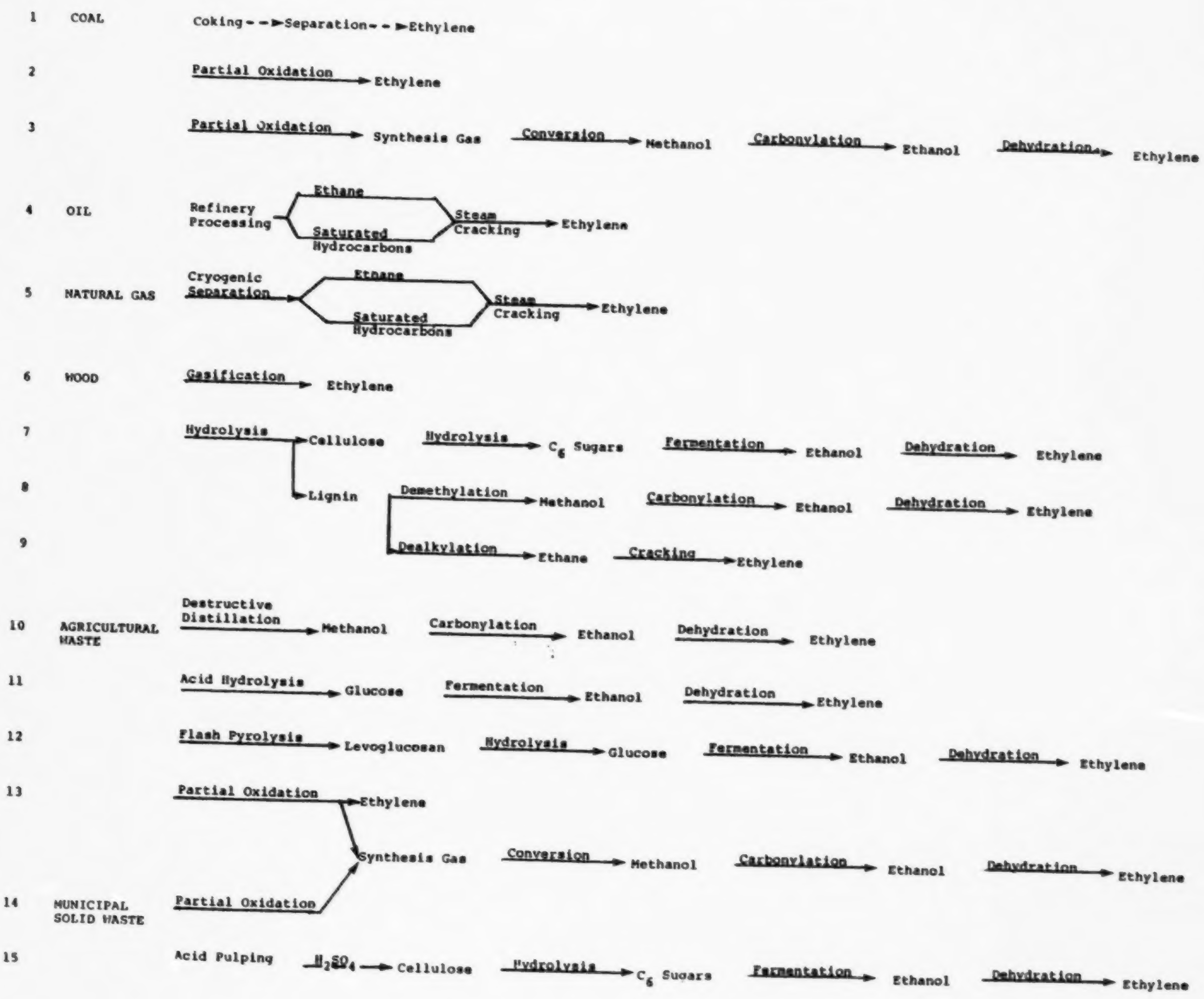
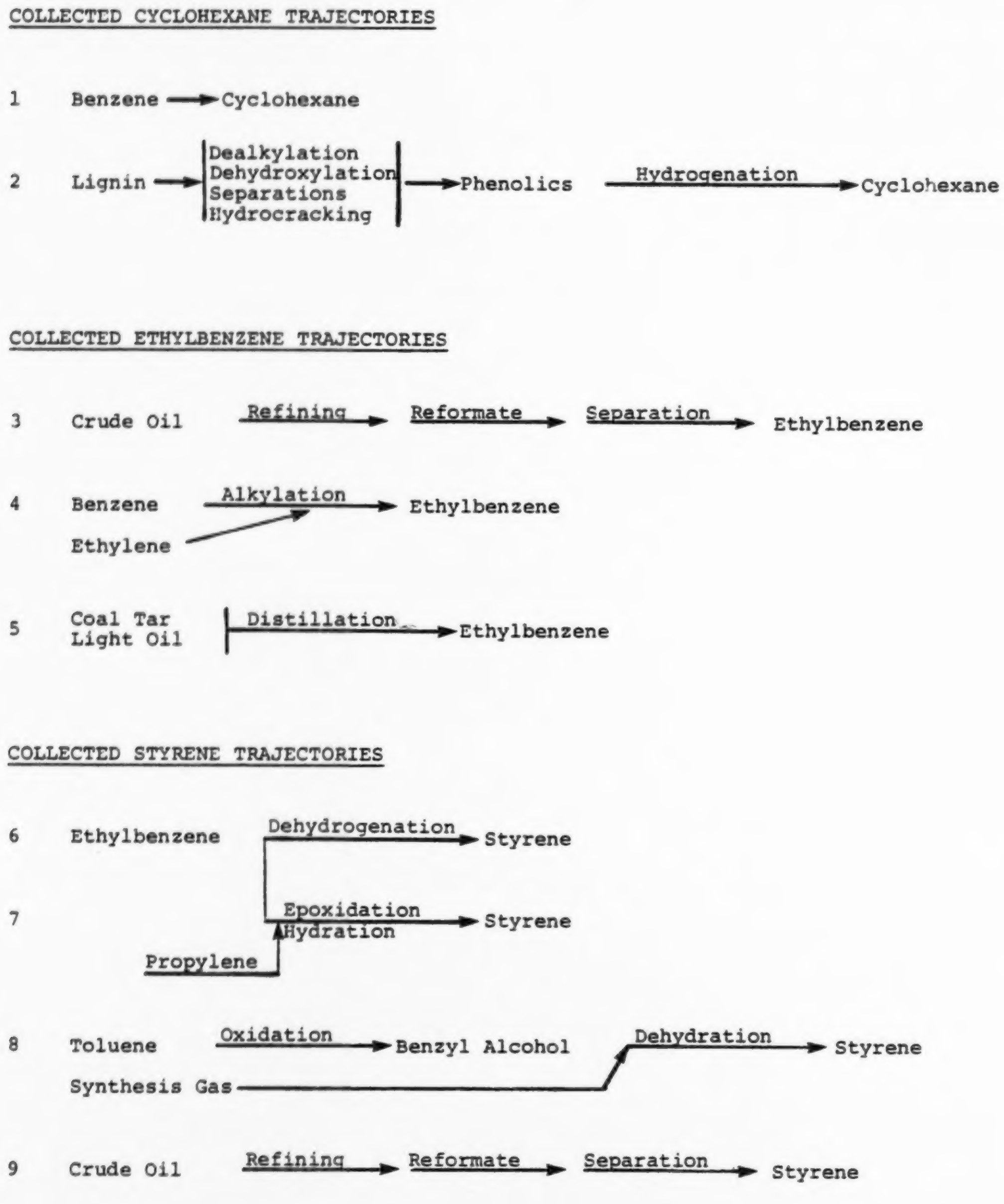

1 COAL Coking - - ►Separation - - ►Ethylene
2 Partial Oxidation → Ethylene
3 Partial Oxidation → Synthesis Gas Conversion → Methanol Carbonylation → Ethanol Dehydration → Ethylene
4 OIL Refinery Processing Ethane Saturated Hydrocarbons Steam Cracking → Ethylene
5 NATURAL GAS Cryogenic Separation Ethane Saturated Hydrocarbons Steam Cracking → Ethylene
6 WOOD Gasification → Ethylene
7 Hydrolysis → Cellulose Hydrolysis → C_6 Sugars Fermentation → Ethanol Dehydration → Ethylene
8 Lignin Demethylation → Methanol Carbonylation → Ethanol Dehydration → Ethylene
9 Dealkylation → Ethane Cracking → Ethylene
10 AGRICULTURAL WASTE Destructive Distillation → Methanol Carbonylation → Ethanol Dehydration → Ethylene
11 Acid Hydrolysis → Glucose Fermentation → Ethanol Dehydration → Ethylene
12 Flash Pyrolysis → Levoglucosan Hydrolysis → Glucose Fermentation → Ethanol Dehydration → Ethylene
13 Partial Oxidation → Ethylene
Synthesis Gas Conversion → Methanol Carbonylation → Ethanol Dehydration → Ethylene
14 MUNICIPAL SOLID WASTE Partial Oxidation
15 Acid Pulping H_2SO_4 → Cellulose Hydrolysis → C_6 Sugars Fermentation → Ethanol Dehydration → Ethylene

Figure E.3. Cyclohexane, Ethylbenzene, Styrene Trajectories


COLLECTED CYCLOHEXANE TRAJECTORIES
1
Benzene
Cyclohexane
2
Lignin
Dealkylation
Dehydroxylation
Separations
Hydrocracking
Phenolics
Hydrogenation
Cyclohexane
COLLECTED ETHYLBENZENE TRAJECTORIES
3
Crude Oil
Refining
Reformate
Separation
Ethylbenzene
4
Benzene
Ethylene
Alkylation
Ethylbenzene
5
Coal Tar
Light Oil
Distillation
Ethylbenzene
COLLECTED STYRENE TRAJECTORIES
6
Ethylbenzene
Dehydrogenation
Styrene
7
Epoxidation
Hydration
Styrene
Propylene
8
Toluene
Oxidation
Benzyl Alcohol
Dehydration
Styrene
Synthesis Gas
9
Crude Oil
Refining
Reformate
Separation
Styrene

percent coming from coal coking. Thus, for analytical purposes the only relevant trajectories shown in Figure E.1 are numbers three and four.

Trajectory four involves four basic processes:

- crude oil refining to pyrolysis gasoline and reformate;
- distillation of refinery products to BTXs;
- distillation of BTX mixture directly to benzene and also to toluene; and
- dealkylation of toluene to benzene.

Of these four, the first -- crude oil refining -- cannot be logically related to the manufacture of benzene or of any chemical. Refineries are built to process fuels and only secondarily to produce chemicals. Thus in terms of environmental impact assignment, this process is irrelevant.

The remaining processes are generally considered in combined form in the existing literature. The major environmental impact from the combined distillation and dealkylation processes involves emission of hydrocarbons (6). Hydrocarbons escape as fugitive emissions from the process units, ancillary equipment, and from plant flares. In the separation and refinement of benzene, a typical refinery emits 0.025 kg of hydrocarbons per kg mole of benzene product (3).

Trajectory number four describes the distillation of light oil derived from the coking of coal to obtain benzene. Around four percent of total consumption is satisfied through this pathway. Benzene production by this trajectory involves two processes:

- coking to obtain light oil; and
- distillation of light oil to benzene.

Since the coking of coal is a process intimately tied to the steel industry and to coke as the primary product, the coking process itself cannot be attributed environmentally to the production of benzene. Light oil is strictly a by-product. Consequently, the entire contribution of residuals relating directly to chemical production results from the distillation process. The significant residuals emitted at this stage are hydrocarbons (3). This process is analogous to the distillation of reformate to BTX in the oil trajectory; therefore, the same coefficients may be applied.

(b) Ethylene. All ethylene consumed in the United States today is derived from petroleum and natural gas. Thus, the only relevant trajectory for environmental impact analysis shown in Figure E.2 is number three.

Within this trajectory there are two main processes:

- refinery processing that liberates ethane and other saturated aliphatic hydrocarbons; or
- separation of natural gas liquids; and
- steam cracking of the hydrocarbons to produce ethylene.

As with benzene, refinery processing is mainly concerned with the production of fuels, with chemicals as a secondary product. Therefore only the cracking process is relevant for analysis of impacts associated with chemical production. Cracking itself contributes only hydrocarbons to the residual stream. The magnitude of emissions due to ethylene production amounts to 0.015 kg of hydrocarbons per kg mole ethylene produced (3).

(c) Cyclohexane. One hundred percent of the cyclohexane manufactured in the United States comes ultimately from petroleum and, specifically, from the hydrogenation of benzene.

Residuals associated with the production of cyclohexane from benzene are nil (6), other than those associated with the production of benzene. The pertinent cyclohexane trajectory is diagrammed in Figure E.3, number one.

(d) Ethylbenzene. One hundred percent of the ethylbenzene consumed in the United States today is derived from petroleum. The two trajectories by which ethylbenzene is manufactured are shown in Figure E.3, numbers three and four.

In trajectory number three, ethylbenzene is essentially a by-product of the distillation of mixed xylenes from refinery reformate. This trajectory is relatively unimportant since it contributes only about eight percent to the total ethylbenzene output.

The main route to ethylbenzene is shown in trajectory number four. This represents the coupling of ethylene to benzene via an alkylation reaction (6). The main residual outflow from this process consists of hydrocarbons (3, 6). Once again these are the result of fugitive emissions from the process unit and from plant flares. The magnitude of hydrocarbon emissions from a typical ethylbenzene plant is 0.051

kg per kg mole ethylbenzene produced (3).

(e) Styrene. Close to one hundred percent of all styrene production in the United States is based on petroleum. Pertinent production processes are pictured in Figure E.3, numbers six, seven, and nine.

Trajectory six represents the major pathway to styrene as employed in the United States. This process consists of dehydrogenation of ethylbenzene to styrene (6).

Trajectory seven shows another pathway through which ethylbenzene is converted to styrene. In this case, propylene is added to ethylbenzene and the mixture is epoxidized. The resulting products are propylene oxide and phenylethyl alcohol. Phenylethyl alcohol is then dehydrated to styrene.

The significant residuals of both processes are hydrocarbons alone. Emissions due to styrene production in both cases amount to 0.042 kg per kg mole styrene produced (3).

Trajectory nine represents the direct distillation of styrene from BTX. Currently, insignificant amounts are produced by this route and it is considered to be environmentally insignificant.

(f) Summary. Table E.1 summarizes the pertinent environmental coefficients associated with the production of the five target chemicals in 1980. As noted, petroleum is currently the major feedstock to all of these chemicals, except ethylene which is coequally fed from natural gas liquids.

Table E.1. R-1980 Relevant Environmental Coefficients

Kg/Kg Mole of Product

TRAJECTORY*	CO	NO_x	SO_2	HYDRO-CARBONS	PARTIC-ULATES	BOD	WASTE SOLIDS/ INDUSTRIAL SLUDGE	ASH
Oil to Benzene(5)	-	-	-	0.025	-	-	-	-
Coal to Benzene(4)	-	-	-	0.025	-	-	-	-
Oil to Ethylene(4)	-	-	-	0.015	-	-	-	-
Cyclohexane(1)	-	-	-	0.051	-	-	-	-
Ethylbenzene(4	-	-	-	Nil	-	-	-	-
Styrene(6)	-	-	-	0.042	-	-	-	-

* Number in parenthesis indicates trajectory number from Figures 9 thru 11.

Source: Council on Environmental Quality. OCS Oil and Gas - An Environmental Assessment: Volume Four. GPO 4000-0035, 1974. pp. IV-1 - IV-24.

Hydrocarbon emissions dominate the residual outflow from each of these production processes. These stem mainly from fugitive emissions and incomplete flare combustion. Insignificant amounts of carbon monoxide, nitrogen oxides, sulfur oxides, particulates, biological oxygen demand, waste solids and ash are generated in the conversion of petroleum to these chemicals. Although refineries do emit appreciable amounts of these residuals, they must logically be attributed to fuel production which accounts for 97 percent of U.S. refinery output.

E.2 R-2000.

As explained in Section 1.3.2, R-2000 represents a "business-as-usual" view of the year 2000. As a consequence, trajectories for the five key chemicals remain essentially the same as in R-1980.

(a) Benzene. In addition to the trajectories outlined in R-1980, 17 percent of benzene demand is provided through coal syngas production. Trajectory number three on Figure E.3 is relevant to this derivation of benzene.

Trajectory number three employs the following processes:

- partial oxidation of coal to synthesis gas; and
- separation of benzene from synthesis gas.

The partial oxidation of coal generates a wide variety of residuals. The magnitudes of these residuals are listed in Table E.2 as a function of benzene production. As with any coal combustion process, CO, NO_x, SO_2, hydrocarbons, par-

Table E.2. R-2000 Relevant Environmental Coefficients

Kg/Kg Mole of Product

Trajectory*	CO	NO_x	SO_2	Hydro-carbons	Partic-ulates	BOD	Waste Solids/ Industrial Sludge	Ash
Oil to Benzene(5)	-	-	-	0.025	-	-	-	-
Coal to Benzene(3)	0.13	1.9	0.9	0.04	0.06	-	16.8	115
Coal to Benzene(4)	-	-	-	0.025	-	-	-	-
Oil to Ethylene(4)	-	-	-	0.051	-	-	-	-
Coal to Ethylene(2)	0.046	0.092	0.348	0.017	0.28	-	7.5	51.4
Cyclohexane(1)	-	-	-	-	-	-	-	-
Ethylbenzene(4	-	-	-	0.051	-	-	-	-
Styrene(6)	-	-	-	0.042	-	-	-	-

* Number in parenthesis indicates trajectory number from Figures 9 thru 11.

Source 1. The Aerospace Corporation. Energy Technologies and the Environment. Environmental Information Handbook. DOE/EV/74010-1, U.S. Dept. of Energy, 1980.

2. Council on Environmental Quality. OCS Oil and Gas - An Environmental Assessment: Volume Four. GPO 4000-0035, 1974. pp. IV-1 - IV-24.

ticulates and ash are generated (1). Additionally, another solid, industrial sludge, is a product of the gas cleaning process used for pollution control. Separation of benzene from synthesis gas does not appear to generate significant quantities of residuals.

(b) Ethylene. In R-2000, coal gasification contributes eight percent to total ethylene demand. Of the three coal-to-ethylene trajectories depicted in Figure E.3, only number two is expected to contribute to this scenario.

The two processes associated with this trajectory are:

- partial oxidation of the coal to gaseous form; and
- separation of ethylene from the product gas.

Partial oxidation is evaluated using the coefficients associated with the Lurgi fixed bed process. This process contributes a variety of residuals to the environment, notably CO, NO_x, SO_2, hydrocarbons, and particulates to the atmosphere and ash and industrial sludge in solid form (1). Alternative processes now in development appear to have much lower potential for environmental impact. The coefficients for the Lurgi residuals are expressed in Table E.2 in kilograms per kg mole of ethylene produced. Separation of product ethylene is not expected to contribute appreciable amounts of any residuals listed in Table E.2 (3).

(c) Cyclohexane. R-1980 coefficients apply for this scenario.

(d) Ethylbenzene. R-1980 coefficients apply for this scenario.

(e) Styrene. R-1980 coefficients apply for this scenario.

(f) Summary. Table E.2 summarizes the environmental coefficients applicable to R-2000. The only major changes are the addition of trajectories to account for the derivation of benzene and ethylene from coal synthesis gas. Cyclohexane, ethylbenzene and styrene remain tied to the processes outlined in R-1980.

E.3. A-1

As described in Section 1.3.3, A-1 is a chemical system in which significant volumes of chemical feedstocks are derived from the gasification of coal and subsequent production of synthesis gas.

(a) Benzene. Forty-seven percent of benzene is derived from coal in this scenario. In Figure E.3, numbers three and four are the relevant trajectories. The R-2000 environmental coefficients for benzene apply for this scenario.

(b) Ethylene. Ethylene is derived from the same process as outlined in R-2000, and the same coefficients apply.

(c) Cyclohexane. R-1980 applies in terms of environmental coefficients.

(d) Ethylbenzene. R-1980 applies in terms of environmental coefficients.

(e) Styrene. In addition to the trajectories outlined in R-1980, trajectory number eight from Figure E.3 is added to satisfy thirty percent of overall styrene demand. This trajectory combines toluene and synthesis gas to obtain styrene in three steps (7):

- oxidation of toluene to benzyl alcohol;
- carbonylation of the benzyl alcohol to phenylethyl alcohol; and
- dehydration of phenylethyl alcohol to styrene.

Oxidation of toluene to benzyl alcohol is accomplished in a single step through a new process developed jointly by the Japanese government and the Sanko Chemical Company. This process is not yet operational, and residual flows have not been characterized (7). Carbonylation of benzyl alcohol to phenylethyl alcohol with synthesis gas is a catalytic process that is also new. Residuals for this process have also not been characterized.

Dehydration of ethylbenzene to styrene takes place in the same manner as in R-1980; therefore, those environmetnal coefficients apply here as well.

(f) Summary. Scenario A-1 adds one new trajectory to styrene. Styrene manufacture does not involve combustion and is not expected to add as much to the residual total as does benzene. The principal processes are not commercially operative at present, however, and have not been definitively characterized in terms of residuals. Table E.3 summarizes relevant environmental coefficients associated with scenario A-1.

Table E.3. A-1 Relevant Environmental Coefficients

Kg/Kg Mole of Product

TRAJECTORY*	CO	NO_x	SO_2	HYDRO-CARBONS	PARTIC-ULATES	BOD	WASTE SOLIDS/ INDUSTRIAL SLUDGE	ASH
Oil to Benzene(5)	-	-	-	0.025	-	-	-	-
Coal to Benzene(3)	0.13	1.9	0.9	0.04	0.06	-	16.8	115
Coal to Benzene(4)	-	-	-	0.025	-	-	-	-
Oil to Ethylene(4)	-	-	-	0.015	-	-	-	-
Coal to Ethylene(2)	0.046	0.92	0.348	0.017	0.28	-	7.5	51.4
Cyclohexane(1)	-	-	-	Nil	-	-	-	-
Ethylbenzene(4	-	-	-	0.051	-	-	-	-
Styrene(6)(8)	-	-	-	0.042	-	-	-	-

* Number in parenthesis indicates trajectory number from Figures 9 thru 11.

Source 1. The Aerospace Corporation. Energy Technologies and the Environment. Environmental Information Handbook. DOE/EV/74010-1, U.S. Dept. of Energy, 1980.

2. Council on Environmental Quality. OCS Oil and Gas - An Environmental Assessment: Volume Four. GPO 4000-0035, 1974. pp. IV-1 - IV-24.

E.4. A-2

This scenario is concerned with the effect of a major synfuels effort on the chemical industry. The most significant impact foreseen occurs with respect to ethylene. As envisioned in A-2, 750 million kg moles, or nearly 70 percent of total consumption, will be generated directly as a by-product of the synfuels industry. Since synfuels will be developed entirely on the basis of their fuel value, the environmental effects of synfuels operations are not assigned here in any part to ethylene production.

Benzene is also produced as a synfuels by-product, although of lesser importance than ethylene. Here, too, environmental effects are attributed to the principal fuel products.

Cyclohexane, ethylbenzene and styrene will continue to be manufactured by the same production trajectories outlined in R-2000. Table E.4 summarizes relevant environmental coefficients associated with Scenario A-2.

E.5. A-3

A-3 looks at a situation in which petroleum is virtually eliminated from use as a major chemical feedstock. Coal and wood supply the feedstocks to satisfy the demand for all but one of the five target chemicals. This scenario employs a number of new trajectories, each of which is discussed below.

(a) Benzene. According to A-3, 90 percent of benzene demand will be met using wood as a feedstock. The remaining

Table E.4. A-2 Relevant Environmental Coefficients

Kg/Kg Mole of Product

Trajectory*	CO	NO_x	SO_2	Hydro-carbons	Partic-ulates	BOD	Waste Solids/ Industrial Sludge	Ash
Oil to Benzene(5)	-	-	-	0.025	-	-	-	-
Coal to Benzene(3)	0.13	1.9	0.9	0.04	0.06	-	16.8	115
Coal Coking to Benzene(4)	-	-	-	0.025	-	-	-	-
Synfuels to Benzene(3)	-	-	-	0.025	-	-	-	-
Oil to Ethylene(4)	-	-	-	0.015	-	-	-	-
Coal to Ethylene(2)	0.046	0.92	0.348	0.017	0.28	-	7.5	51.4
Synfuels to Ethylene**	-	-	-	Nil	-	-	-	-
Cyclohexane(1)	-	-	-	Nil	-	-	-	-
Ethylbenzene(4	-	-	-	0.051	-	-	-	-
Styrene(6)	-	-	-	0.042	-	-	-	-

* Number in parenthesis indicates trajectory number from Figures 9 thru 11.

** Ethylene is a by-product of the synfuels industry. Residuals incurred are due to fuel processing activities.

Source 1. The Aerospace Corporation. Energy Technologies and the Environment. Environmental Information Handbook. DOE/EV/74010-1, U.S. Dept. of Energy, 1980.

2. Council on Environmental Quality. OCS Oil and Gas - An Environmental Assessment: Volume Four. GPO 4000-0035, 1974. pp. IV-1 - IV-24.

ten percent will come through coal light oil distillation (trajectory number four, Figure E.1). Petroleum will cease to be a feedstock for benzene and other aromatics.

Wood is converted into benzene by a series of four processes as diagrammed in Figure E.1, trajectory number six:

- o hydrolysis to reduce the wood to cellulose and lignin;
- o purification of the hydrolysis product;
- o fragmentation of lignin into basic aromatic structures (phenolics); and
- o treatment of phenolics to yield benzene.

Breaking down the complex structure of wood into lignin and cellulose through fragmentation and separation, or delignification, is a well characterized process, being one of the basic processes currently used in the paper industry. Residuals associated with this process should be nil except for particulates generated by wood chipping in the preparation phase (4). This activity generates around 0.018 kg of particulates per kg mole of benzene produced (2).

The purification process that effectively separates lignin from cellulose is not expected to contribute significant residuals to the environment (4).

The third process in this trajectory is not well defined in the technical literature. There are no current industrial methods for converting lignin to phenolics. As a result, no residual coefficients can be calculated for this process.

The last stage of processing involves conversion of the various phenolic components derived from lignin degradation to benzene. Due to a vast array of possibilities with respect to product mix, it is impossible to decide which process type will dominate this conversion step. Product mix will depend on the type of tree used and on the method of lignin degradation chosen. Depending on the form of this product mix, phenolics can be converted to benzene and related products by dealkylation, dehydroxylation, separation or hydrocracking. Therefore, since the process is unclear, it is not possible to identify a residual stream with any degree of accuracy.

(b) Ethylene. A-3 satisfies ethylene demand through six routes, represented by trajectories four through nine in Figure E.2.

Trajectories four and five are standard petrochemical processes already discussed in R-1980, with the same residual coefficients applying.

Trajectory six represents wood gasification, which in this scenario satisfies a very small portion of total estimated ethylene demand and is considered insiginificant.

Trajectory seven involves five major processes. They are:

- hydrolysis of wood to lignin and cellulose;
- separation of the lignin and cellulose;
- hydrolysis of the cellulose to fermentable C_6 sugars;
- fermentation of the C_6 sugars to ethanol; and
- dehydration of the ethanol to ethylene.

The first two processes have the same residual coefficients as the wood-to-benzene trajectory discussed earlier.

Hydrolysis of the cellulose to C_6 sugars is an enclosed process and insignificant amounts of residuals are expected to escape either to water or to the atmosphere (4).

Fermentation of the C_6 sugars to ethanol is expected to emit hydrocarbons at about 0.106 kg per kg mole of ethylene produced (4). Liquid residue from the fermentation will contribute a biological oxygen demand, after plant secondary treatment, of 0.57 kg per kg mole of ethylene produced (2). This is the amount of BOD expected to remain in liquids released at the plant boundary to municipal sewer systems. However, it is our opinion that these plants are likely to be located in remote areas without such service. In that case, complete treatment would have to be undertaken within plant boundaries. Depending on the technical state of treatment technology and future water quality criteria, this BOD value could approach zero.

Waste solids from the beer stills and rectifying columns are generated at a rate of 5.4 kg per kg mole of ethylene produced (2). These solids have high BOD and are currently processed into cattle feed or disposed of in landfills.

Ethanol dehydration to ethylene is also an enclosed process. Quench water used in the process is continually recycled, and is not emitted to the environment. Residuals attributable to this processing phase are considered insignificant (5).

Trajectory eight utilizes lignin as a feedstock to obtain ethylene. There are five processees involved in this trajectory.

- hydrolysis of wood to lignin and cellulose;
- separation of lignin and cellulose;
- demethylation of the lignin to produce methanol;
- carbonylation of the methanol to ethanol; and
- dehydration of ethanol to ethylene.

Again, the first two processes and associated residual coefficients are the same as in the wood-to-benzene trajectory presented earlier.

The third process has never been employed commercially for the conversion of lignin to methanol. Residual flows are not characterized and coefficients are not derivable at this time.

The fourth process is a carbonylation reaction from which hydrocarbons can be expected to escape as fugitive emissions. These amounts are expected to be minor and are an insignificant contribution to the environment. Dehydration to ethylene also is not expected to contribute significant amounts of residuals (3).

Trajectory eight involves four processes to derive ethylene from lignin. They are:

- hydrolysis of wood to lignin and cellulose;
- separation of cellulose and lignin;
- dealkylation of lignin to ethane; and
- cracking of ethane to ethylene.

The first two processes are the same as those converting wood into benzene, with the same environmental coefficients.

Residuals from the dealkylation process will vary with the structure of lignin used as the feed. The lignin structure varies significantly among hard and softwoods and other biomass, and somewhat between species of tree. Thus, it is not possible to characterize residual flows for this process.

Cracking ethane to ethylene is a process widely utilized in the petroleum refining industry. Ethane cracking produces only hydrogen gas and water condensate along with other hydrocarbons that are recovered and not considered residuals. Hydrogen gas is recycled to produce steam or used in other reforming plants. Fugitive hydrocarbons emitted form the process are insignificant (3).

(c) Cyclohexane. The entire demand for cyclohexane is satisified through biomass in Scenario A-3. Cyclohexane is derived through trajectory number two shown in Figure E.3. This trajectory involves four processes:

- Hydrolysis of wood to lignin and cellulose;
- separation of lignin from product mixture;
- dehydroxylation, dealkylation, separation and hydrocracking to derive phenolics; and
- hydrogenation of phenolics to cyclohexane.

The first two processes are the same as those described for the wood-to-benzene trajectory. The third process contributes an unknown array of residuals for a variety of processes, selected depending on the nature of the lignin used.

Hydrogenation of phenolics to cyclohexane is not an established industrial process. Residual flows will depend on process parameters that have not been established.

(d) Ethylbenzene. Ethylbenzene continues to be derived using the same methods as in R-2000.

(e) Styrene. Styrene continues to be derived using the same methods as in R-2000.

(f) Summary. A-3 involves a large scale shift in chemical feedstocks from petroleum and natural gas to biomass. Many of the processes used in feedstock conversion are speculative and theoretical in nature. Lignin chemistry is especially lacking and the lignin chemical structure will vary considerably, depending on the biomass source. Since processing to chemicals depends on structure for the proper choice of reagents and reaction conditions, and since there are no current industrial processes using lignin as a feedstock to chemicals, residuals from these processes cannot be characterized or determined. From an environmental standpoint, however, it seems apparent that if any significant residuals occur, they will probably be hydrocarbons emitted to the atmosphere.

Cellulose conversion to sugars and their subsequent conversion to ethanol is well characterized in the technical literature. Residuals here are high in BOD and solids. Table E.5 summarizes relevant environmental coefficients associated with scenario A-3.

Table E.5. Relevant Environmental Coefficients

Kg/Kg Mole of Product

TRAJECTORY*	CO	NO_x	SO_2	HYDRO-CARBONS	PARTIC-ULATES	BOD	WASTE SOLIDS/ INDUSTRIAL SLUDGE	ASH
Coal Coking to Benzene(4)	-	-	-	0.025	-	-	-	-
Biomass to Benzene(6)	?	-	-	?	0.018	-	-	-
Oil to Ethylene(4)	-	-	-	0.015	-	-	-	-
Biomass to Ethylene(7)	-	-	-	0.106	0.006	0.57	5.4	-
Biomass to Cyclohexane(2)	?	-	-	?	-	-	-	-
Ethylbenzene(4	-	-	-	0.051	-	-	-	-
Styrene(6)	-	-	-	0.042	-	-	-	-

* Number in parenthesis indicates trajectory number from Figures 9 thru 13.

Source 1. The Aerospace Corporation. Energy Technologies and the Environment. Environmental Information Handbook. DOE/EV/74010-1, U.S. Dept. of Energy, 1980.

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F.1. Fossil Hydrocarbon Derived Feedstocks

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C.2. Biomass Derived Feedstocks

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Paper covers the potential of biomass as a substitute for petroleum as a feedstock to the chemical industry using a quantitative methodology. Economic feasibility and the conversion processes of biomass chemicals are charted and discussed. Petroleum savings associated with feedstock changeover are assessed. Outlook for chemicals from biomass at the turn of the century is summarized.

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Smith, N. Wood: An Ancient Fuel with a New Future. World Watch Paper 42, Worldwatch Institute, Washington, DC, 1981. 48 pp.

A comprehensive look at the development of wood as an energy source to displace petroleum. Environmental impacts of large scale biomass production are discussed.

Society of American Foresters. 10th Annual Spring Symposium for the Florida Section. Energy From Forestry, Production and Use. 1978.

Examination of the impact of silviculture on farmland, including nutrient depletions and fertilizer requirements.

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Article deals with the production, availability and conversion potential of biomass into useful commodities.

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Article examines the production possibilities and consumption trends of the forest products industry. Wood as a chemical raw material is considered with various conversion possibilities outlined.

Stokes, C.A., and G.D. Waterland. Alcohols: The Old New Fuels. Technology Review, July 1981. pp. 68-79.

Prospects for large scale production and use of methanol and ethanol by the end of the century.

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Report contains information regarding the degradation of cellulosic materials to sugars via microbiological means. Also covered are new fermentation processes for the conversion of sugars so obtained to acrylic acid, butanol, acetic acid, and ethanol which are important feedstocks for the chemical industry. All procedures covered are laboratory bench scale in magnitude. No industrial application of this technology is noted.

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Possible sources of biomass are described in terms of their productive capacities.

Weiss, L.H., and C.J. Mikulka. Gasohol: A Realistic Assessment. Preprint of a presentation to the 89th National Meeting of the American Institute of Chemical Engineers. Chem Systems Inc, New York, 1980.

Article contains information on the ethanol production capacity of the United States, including projections as a function of corn, sweet sorghum and cellulosic feedstocks availability. The economics of all aspects of the production process are given. Both supply limited and maximum growth cases are considered.

Weiss, L.H. Ethylene from Biomass. Preprint for the 89th National Meeting of the American Institute of Chemical Engineers. Chem Systems Inc, New York, August 1980.

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Biomass farms require high quality land to maximize energy yield and minimize environmental hazards. The shortage of such land may hinder development of energy farms. Most of 760 million acres of classes I-IV rural land would need considerable measures to overcome inherent development problems.

C.2.2. Related Sources

Ann Arbor Science Publishers
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Chemicals From Western Hardwoods and Agricultural Residues, Annual Report. PB80-118474.

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Silviculture Biomass Farms.
  V. Conversion Processes and Costs. Technical Report 7347
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System Study of Fuels From Sugarcane,.... Vol. 3. Conversion to Fuels and Chemical Feedstocks. BMT 1957, v.3.

C.3. Chemical Industry Information

Anderson, E.V. Economics Favor U.S. Trade in Chemicals. Chemical and Engineering News, December 22, 1980. pp. 33-35.

> U.S. chemical manufacturers will continue to maintain a strong position in world markets, despite trade disputes with EEC countries. A healthy trade surplus is expected to continue in the near future.

Anderson, J.D. Aromatics Supply in the 1980's. Chemical and Engineering Progress, December 1980. pp. 39-42.

> Chemical demand for aromatics in the next several years will be satisfied due to decreasing fuel use demand.

Anonymous. New Plants and Facilities. C.E. Construction Alert. Chemical Engineering, October 20, 1980. pp. 121-135.

> Location, capacities and ownership of new chemical manufacturing projects announced from January to August 1980 are listed in tabular form.

Anonymous. Petrochemical Feedstock Issues Aired. Oil and Gas Journal, July 2, 1979. p. 70.

> As the demand for fuel use hydrocarbons rises, the availability of economical feedstocks for the chemical industry decreases. As oil prices continue to be bid up by fuel users, the U.S. competitive advantage in the world chemical markets will diminish or disappear.

Anonymous. U.S. Petrochemical Feed Seen Adequate through 1985. Oil and Gas Journal, October 1, 1979. p. 49.

> The petrochemical industry will use little feedstock from sources other than oil through 1985.

Anonymous. U.S. Petrochemical Feed Supply in Danger. Oil and Gas Journal, July 23, 1979. pp. 38-39.

> Government policies mandating the use of petroleum for fuel uses may pose a threat to feedstock allocations for the chemical industry.

Anonymous. Shell Ethylene View 4.3%. Chemical Marketing Reporter, January 5, 1981. p. 3.

> World ethylene demand is expected to increase by 4.3 percent per year over the next 20 years with a net increase in consumption of 100 billion pounds.

Anonymous. Raw Material Shifts in U.S. Chemicals to Come Downstream from Basic Feeds. Chemical Marketing Reporter, October 13, 1980. p. 5.

> Any significant shifts in feedstock by the U.S. chemical industry over the next twenty years will most likely come in the stages of production after basic olefins and aromatics which are themselves feedstocks.

Carmichael, J. Chemicals. Forbes, January 5, 1981. pp. 198-199.

> American competitive edge in petrochemical production may erode as Middle Eastern countries enter the petrochemical manufacturing industry.

CEQ. OCS Oil and Gas - An Environmental Assessment: Volume four. GPO 4000-035, Council on Environmental Quality, 1974. pp. IV-1--IV-24.

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Considine, D.M. Chemical and Process Technology Encyclopedia. Petrochemical Complex. McGraw-Hill, New York, 1974. pp. 841-848.

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> Excellent overview of the use of synthetics, petrochemical sources, natural material alternates, alternate feed sources, and how these may interact in the future with respect to demand use and supply.

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> Facts and figures on air and water pollution sources.

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> Contains descriptions of processes that occur in the petroleum refining complex. Waste streams and control technology associated with these waste streams are discussed in connection with each outlined process.

Klein, R.A. Olefin Feedstocks: A Fat-Free Diet for Industry. Chemical and Engineering Progress, December 1980. pp. 34-35.

> Industry will continue to move toward heavier feedstocks for ethylene production as economics dictate such shifts.

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Liepins, R., et al. Industrial Process Profiles for Environmental Use: Chapter 6. The Industrial Organic Chemical Industry. EPA-600/2-77-023E, PB-281478, U.S. Environmental Protection Agency, Research Triangle Park, NC, February 1977. 992 pp.

> Organic chemical manufacturing processes are discussed in terms of ten feedstock groups of which benzene and ethylene are members. Groups are further broken down into production processes utilizing these feedstocks, and their environmental effects are discussed.

Mannsville Chemical Products. Chemical Products Synopsis. Cortland, NY.

Menchin, W.R. Envrionmental Impacts Efficiency and Cost of Energy Supply and End Use. Volumes one and two. Hittman Associates, Inc. Columbia, MD, 1974.

> Quantitative information on the residuals of coal processing technologies (gasification and liquefaction) is presented. Residual streams associated with discrete processes are given.

Schneider, S.A. Common Sense About Energy, Part One: Where Has All the Oil Gone? Working Papers, January/February 1978. pp. 31-42.

Exploitation of coal reserves in an effort to gain energy independence will increase the amount of gaseous pollutants discharged into the air. Sulfur dioxide from a single coal-fired plant causes about 25 fatalities, 60,000 cases of respiratory disease and 12 million dollars in property damage each year.

Sneath, W.S. Petrochemicals: A Natural for the '80's. Chemical and Engineering Progress, December 1980. pp. 44-49.

Synthetics will continue to provide net energy savings to manufacturing industries (i.e., auto, plumbing, fabric). The inherent ability of the petrochemical complex to shift to accommodate new feedstocks to provide basic chemicals will ensure an adequate supply of these materials in the face of rising oil prices.

USEPA. Economic Impact of EPA's Regulations on the Petroleum Industry. Parts one, two and three. EPA-230/3-76-004, U.S. Environmental Protection Agency, Washington, DC, 1976.

Petrochemical complex description with process residual streams identified. Abatement procedures are discussed with the economic implications of abatement.

USEPA. Environmental Outlook 1980. EPA 600/8-80-003, U.S. Environmental Protection Agency, Office of Research and Development, Washington, DC, 1980.

Forecasts of total pollutant emissions and sources into the year 2000 with comparison to 1975 emissions. Health effects of pollutants are discussed.

Weaver, W.C. Meeting the Olefin Demand 1980-2000. Chemical and Engineering Progress, December 1980. pp. 31-33.

Several firms are developing processes to utilize heavier residual oil as feeds to olefin production. When these plants become operational, ethylene will be coming from the full range of petroleum sources. Petroleum will continue to be the best source of olefin feedstocks through the rest of the century.

Weismantel, G.E. Feedstocks vs. Gasoline: What will Happen Next? Chemical Engineering, August 25, 1980. pp. 37-39.

> Unleaded gasoline requires addition of BTX compounds to increase its octane rating without the use of lead. With the phase-out of leaded premium gasolines, high BTX content unleaded premiums will enter the market, tightening the supply of BTX from petroleum sources.

Wishart, R.S. Industrial Energy in Transition: A Petrochemical Perspective. Science, February 10, 1978. pp. 614-18.

> Article concentrates on improving the efficiency of petroleum use in the petrochemcial industry. New technologies are mentioned. Coal as a feedstock is also explored and its limitations discussed. Synthesis gas production from coal is given much promise. Biomass is expected to be a contributor to the chemical industry by 2000. A contribution to the total feedstocks requirement of 10 to 15 percent is expected by the year 2000 through the use of coal and biomass.

Word, T.T. Where Will Light Hydrocarbon Feedstocks Fit in the 80's? Chemical and Engineering Progress, December 1980. pp. 36-38.

> Although there is an industry-wide trend toward cracking heavier portions of crude oil for ethylene production, light hydrocarbon units are expected to remain operational in the near future.

APPENDIX G. CONVERSION FACTORS

Table G.1. Conversion Factors

Unit	x	Conversion Factor	=	S.I. Unit
Acre		4047		square meters
Barrel		0.1590		cubic meter
BTU		1055		joules
Gallon		0.003785		cubic meter
Metric Ton		1000		kilograms
Quad		1.055×10^{18}		joules
Ton		907.2		kilograms